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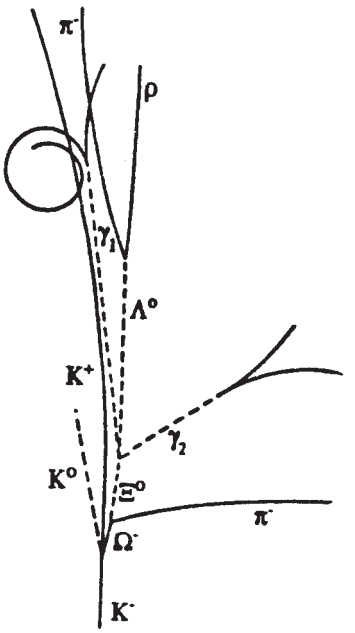

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ON GENERALIZED JORDAN PREDERIVATIONS AND GENERALIZED PREDERIVATIONS OF JORDAN LIE SUPERALGEBRAS

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Abstract

In this paper, the concepts of (generalized) (θ, φ)-prederivations and (generalized) Jordan (θ, φ)-prederivations on a Jordan Lie superalgebra are introduced. It is proved that Jordan (θ, φ)-prederivations (resp. generalized Jordan (θ, φ)-prederivations) are (θ, φ)-prederivations (resp. generalized (θ, φ)-prederivations) on a Jordan Lie superalgebra under some conditions. In particular, Jordan θ-prederivations are θ-prederivations on a Jordan Lie superalgebra.

Key words: Derivations, Prederivations, Jordan Lie superalgebras
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§1 Introduction

Derivations and generalized derivations are interesting subjects both in mathematics and physics, and there has been a great deal of work concerning them. Leger and Luks investigated the structure of the generalized derivations of Jordan Lie algebras systematically (cf. [11]). Generalized derivations on rings was studied in [12, 16]. Generalized derivations also play a key role in Benoist's study of Levi factors in derivation algebras of nilpotent Lie algebras (cf. [3]). In 1969, Herstein showed that a Jordan derivation of a prime ring of characteristic not 2 must be a derivation(cf. [9]). Brešar, M. together with Vukman, J. generalized Herstein's result to Jordan (Θ, φ)-derivations (cf. [4, 5]). In [1], the authors proved that in a 2-torsion free non-commutative prime ring R, a generalized Jordan (θ, φ)-derivation is a generalized (θ, φ)-derivation when θ is an automorphism of R. We gave some results on generalized derivations of Lie color algebras [8]. Moreover, Jordan θ-derivations and generalized Jordan derivations of Lie triple systems were studied in [15–17].

Prederivations (or Lie triple derivations) of Lie algebras were first introduced by Müller to study bi-invariant semi-Riemannian metrics on Lie groups (cf. [14]). Bajo proved that any real or complex Lie algebras admitting a non-singular prederivation is necessarily nilpotent (cf. [2]). In recent years, there has been an increasing interest in investigating prederivations (cf. [6, 7, 10, 12, 13, 18, 20]).

Jordan Lie superalgebras are the natural generalization of Lie superalgebras, and have important applications both in mathematics and physics. Jordan Lie superalgebras are also interesting from a purely mathematical point of view (cf. [19]). In this paper, we introduce the concepts of (generalized) (θ, φ)-prederivations and (generalized) Jordan (θ, φ)-prederivations

for a Jordan Lie superalgebra and obtain some results concerning Jordan (θ,φ)-prederivations (resp. generalized Jordan (θ,φ)-prederivations) and (θ,φ)-prederivations (resp. generalized (θ,φ)-prederivations) on a Jordan Lie superalgebra.

Throughout this paper, the base field $\mathbf{F}$ is assumed to be of characteristic not equal to 3. We now recall some elementary definitions.

§2 Concepts

Definition 2.1. [19] Let L be a $\mathbf{Z_2}$-graded vector space,i.e., $L = L_0 \oplus L_1$ with grading function $d(x)$ give by$d(x) = 0, x \in L_0; d(x) = 1, x \in L_1$. Suppose that a bilinear product $[.,.] : L \otimes L \to L$ satisfies conditions

(i) $d([x,y]) = \{d(x) + d(y)\} \pmod 2$,

(ii) $[y,x] = -\delta(-1)^{d(x)d(y)}[x,y]$,

(iii) $(-1)^{d(x)d(z)}[[x,y],z]+(-1)^{d(y)d(x)}[[y,z],x]+(-1)^{d(z)d(y)}[[z,x],y] = 0$.

We call L a Jordan Lie superalgebra. Clearly, The case of $\delta = 1$ gives the Lie superalgebra.

Definition 2.2. A prederivation (Lie triple derivation) of a Jordan Lie superalgebra L is a linear mapping $D : L \to L$ such that $D([[x,y],z]) = [[D(x),y],z] + [[x,D(y)],z] + [[x,y],D(z)], \forall x,y,z \in L$.

Definition 2.3. A Jordan prederivation (Jordan triple derivation) of a Jordan Lie superalgebra L is a linear mapping $D' : L \to L$ such that $D'([[x,y],x]) = [[D'(x),y],x] + [[x,D'(y)],x] + [[x,y],D'(x)], \forall x,y,z \in L$.

Definition 2.4. Let L be a Jordan Lie superalgebra and let $D,\theta,\varphi : L \to L$ be homogeneous linear mappings, where $d(\theta) = d(\varphi) = 0$. We denote by $d(D)$ the $\mathbf{Z_2}$-graded degree of a homogeneous linear mapping D of L.

1. D is called a $(\theta,\varphi)_1$**-prederivation** if

$$\begin{aligned} D([[x,y],z]) =& [[D(x),\theta(y)],\varphi(z)] + (-1)^{d(D)d(x)}[[\theta(x),D(y)],\varphi(z)] \\ &+ (-1)^{d(D)(d(x)+d(y))}[[\theta(x),\varphi(y)],D(z)], \forall x,y,z \in L. \end{aligned}$$

2. D is called a $(\theta,\varphi)_2$-**prederivation** if

$$\begin{aligned}D([[x,y],z]) =&[[D(x),\theta(y)],\theta(z)]+(-1)^{d(D)d(x)}[[\theta(x),D(y)],\varphi(z)]\\&+(-1)^{d(D)(d(x)+d(y))}[[\varphi(x),\varphi(y)],D(z)],\forall x,y,z\in L.\end{aligned}$$

3. D is called a $(\theta,\varphi)_3$-**prederivation** if

$$\begin{aligned}D([[x,y],z]) =&[[D(x),\theta(y)],\theta(z)]+(-1)^{d(D)d(x)}[[\varphi(x),D(y)],\theta(z)]\\&+(-1)^{d(D)(d(x)+d(y))}[[\varphi(x),\varphi(y)],D(z)],\forall x,y,z\in L.\end{aligned}$$

In particular, a $(\theta,\varphi)_i$-prederivation D is called a θ-**prederivation** if $\theta=\varphi$, $\forall i=1,2,3$. It is clear that a $(\theta,\varphi)_i$-prederivation is a prederivation when $\theta=\varphi=1_T$.

Definition 2.5. Let L be a Jordan Lie superalgebra and let $D,\theta,\varphi: L\to L$ be homogeneous linear mappings, where $d(\theta)=d(\varphi)=0$.

1. D is called a **Jordan** $(\theta,\varphi)_1$-**prederivation** if

$$\begin{aligned}D([[x,y],x]) =&[[D(x),\theta(y)],\varphi(x)]+(-1)^{d(D)d(x)}[[\theta(x),D(y)],\varphi(x)]\\&+(-1)^{d(D)(d(x)+d(y))}[[\theta(x),\varphi(y)],D(x)],\forall x,y\in L.\end{aligned}$$

2. D is called a **Jordan** $(\theta,\varphi)_2$-**prederivation** if

$$\begin{aligned}D([[x,y],x]) =&[[D(x),\theta(y)],\theta(x)]+(-1)^{d(D)d(x)}[[\theta(x),D(y)],\varphi(x)]\\&+(-1)^{d(D)(d(x)+d(y))}[[\varphi(x),\varphi(y)],D(x)],\forall x,y\in L.\end{aligned}$$

3. D is called a **Jordan** $(\theta,\varphi)_3$-**prederivation** if

$$\begin{aligned}D([[x,y],x]) =&[[D(x),\theta(y)],\theta(x)]+(-1)^{d(D)d(x)}[[\varphi(x),D(y)],\theta(x)]\\&+(-1)^{d(D)(d(x)+d(y))}[[\varphi(x),\varphi(y)],D(x)],\forall x,y\in L.\end{aligned}$$

In particular, $\forall i = 1, 2, 3$, a Jordan $(\theta, \varphi)_i$-prederivation D is called a **Jordan θ-prederivation** if $\theta = \varphi$. It is clear that a Jordan $(\theta, \varphi)_i$-prederivation is a Jordan prederivation when $\theta = \varphi = 1_T$.

It is clear that if D_i is a $(\theta, \varphi)_i$-prederivation of L, then D_i is a Jordan $(\theta, \varphi)_i$-prederivation of L, where $i = 1, 2, 3$.

In this paper, L is a Jordan Lie superalgebra and θ, φ are defined to be homogeneous linear mappings of L satisfying $d(\theta) = d(\varphi) = 0$.

Definition 2.6. Let L be a Jordan Lie superalgebra.

1. A **generalized $(\theta, \varphi)_1$-prederivation** with respect to a $(\theta, \varphi)_1$-prederivation E_1 is a homogeneous linear mapping $D_1 : L \to L$ such that $d(D_1) = d(E_1)$ and

$$\begin{aligned} D_1([[x, y], z]) =& [[E_1(x), \theta(y)], \varphi(z)] + (-1)^{d(D_1)d(x)}[[\theta(x), E_1(y)], \varphi(z)] \\ &+ (-1)^{d(D_1)(d(x)+d(y))}[[\theta(x), \varphi(y)], D_1(z)], \forall x, y, z \in L. \end{aligned}$$

2. A **generalized $(\theta, \varphi)_2$-prederivation** with respect to a $(\theta, \varphi)_2$-prederivation E_2 is a homogeneous linear mapping $D_2 : L \to L$ such that $d(D_2) = d(E_2)$ and

$$\begin{aligned} D_2([[x, y], z]) =& [[E_2(x), \theta(y)], \theta(z)] + (-1)^{d(D_2)d(x)}[[\theta(x), E_2(y)], \varphi(z)] \\ &+ (-1)^{d(D_2)(d(x)+d(y))}[[\varphi(x), \varphi(y)], D_2(z)], \forall x, y, z \in L. \end{aligned}$$

3. A **generalized $(\theta, \varphi)_3$-prederivation** with respect to a $(\theta, \varphi)_3$-prederivation δ_3 is a homogeneous linear mapping $D_3 : L \to L$ such that $d(D_3) = d(E_3)$ and

$$\begin{aligned} D_3([[x, y], z]) =& [[E_3(x), \theta(y)], \theta(z)] + (-1)^{d(D_3)d(x)}[[\varphi(x), E_3(y)], \theta(z)] \\ &+ (-1)^{d(D_3)(d(x)+d(y))}[[\varphi(x), \varphi(y)], D_3(z)], \forall x, y, z \in L. \end{aligned}$$

In particular, $\forall i = 1, 2, 3$, a generalized $(\theta, \varphi)_i$-prederivation D is called a **generalized θ-prederivation** with respect to a θ-prederivation E if $\theta = \varphi$.

It is clear that D is a generalized prederivation when $\theta = \varphi = 1_T$ and E is a prederivation.

Definition 2.7. Let L be a Jordan Lie superalgebra.

1. A **generalized Jordan $(\theta, \varphi)_1$-prederivation** with respect to a Jordan $(\theta, \varphi)_1$-prederivation E_1 is a homogeneous linear mapping $D_1 : L \to L$ such that $d(D_1) = d(E_1)$ and

$$\begin{aligned} D_1([[x, y], x]) =& [[E_1(x), \theta(y)], \varphi(x)] + (-1)^{d(D_1)d(x)}[[\theta(x), E_1(y)], \varphi(x)] \\ &+ (-1)^{d(D_1)(d(x)+d(y))}[[\theta(x), \varphi(y)], D_1(x)], \forall x, y \in L. \end{aligned}$$

2. A **generalized Jordan $(\theta, \varphi)_2$-prederivation** with respect to a Jordan $(\theta, \varphi)_2$-prederivation E_2 is a homogeneous linear mapping $D_2 : L \to L$ such that $d(D_2) = d(E_2)$ and

$$\begin{aligned} D_2([[x, y], x]) =& [[E_2(x), \theta(y)], \theta(x)] + (-1)^{d(D_2)d(x)}[[\theta(x), E_2(y)], \varphi(x)] \\ &+ (-1)^{d(D_2)(d(x)+d(y))}[[\varphi(x), \varphi(y)], D_2(x)], \forall x, y \in L. \end{aligned}$$

3. A **generalized Jordan $(\theta, \varphi)_3$-prederivation** with respect to a Jordan $(\theta, \varphi)_3$-prederivation E_3 is a homogeneous linear mapping $D_3 : L \to L$ such that $d(D_3) = d(E_3)$ and

$$\begin{aligned} D_3([[x, y], x]) =& [[E_3(x), \theta(y)], \theta(x)] + (-1)^{d(D_3)d(x)}[[\varphi(x), E_3(y)], \theta(x)] \\ &+ (-1)^{d(D_3)(d(x)+d(y))}[[\varphi(x), \varphi(y)], D_3(x)], \forall x, y \in L. \end{aligned}$$

In particular, $\forall i = 1, 2, 3$, a generalized Jordan $(\theta, \varphi)_i$-prederivation D is called a **generalized Jordan θ-prederivation** with respect to a Jordan θ-prederivation E if $\theta = \varphi$. It is clear that D is a generalized Jordan prederivation when $\theta = \varphi = 1_T$ and E is a Jordan prederivation.

§3 Main Results

Theorem 3.1. D is a $(\theta,\varphi)_1$-prederivation of L if and only if D is a Jordan $(\theta,\varphi)_1$-prederivation of L such that

(i) $[[\theta(x),\varphi(y)],D(z)]=[[\varphi(x),\theta(y)],D(z)]$,

(ii) $(-1)^{d(x)d(z)}A(x,y,z)+(-1)^{d(x)d(y)}A(y,z,x)+(-1)^{d(y)d(z)}A(z,x,y)=0$,

where $x,y,z\in L$ and $A(x,y,z)=[[D(x),\theta(y)],\varphi(z)]+(-1)^{d(D)d(x)}[[\theta(x),D(y)],\varphi(z)]+(-1)^{d(D)(d(x)+d(y))}[[\theta(x),\varphi(y)],D(z)]$.

Proof. Assume that D is a $(\theta,\varphi)_1$-prederivation of L. Clearly, D is a Jordan $(\theta,\varphi)_1$-prederivation of L and $D([[x,y],z])=-\delta(-1)^{d(x)d(y)}D([[y,x],z])$; note that

$$\begin{aligned}
&-\delta(-1)^{d(x)d(y)}D([[y,x],z])\\
=&-\delta(-1)^{d(x)d(y)}[[D(y),\theta(x)],\varphi(z)]-\delta(-1)^{d(x)d(y)}(-1)^{d(D)d(y)}[[\theta(y),D(x)],\varphi(z)]\\
&-\delta(-1)^{d(x)d(y)}(-1)^{d(D)(d(x)+d(y))}[[\theta(y),\varphi(x)],D(z)]\\
=&[D(x),\theta(y),\varphi(z)]+(-1)^{d(D)d(x)}[[\theta(x),D(y)],\varphi(z)]\\
&+(-1)^{d(D)(d(x)+d(y))}[[\varphi(x),\theta(y)],D(z)]
\end{aligned}$$

and

$$\begin{aligned}
D([[x,y],z])=&[[D(x),\theta(y)],\varphi(z)]+(-1)^{d(D)d(x)}[[\theta(x),D(y)],\varphi(z)]\\
&+(-1)^{d(D)(d(x)+d(y))}[[\theta(x),\varphi(y)],D(z)],
\end{aligned}$$

then (i) follows. Since D is a $(\theta,\varphi)_1$-prederivation of L, we have $D([[x,y],z])=A(x,y,z)$; hence

$$\begin{aligned}
&(-1)^{d(x)d(z)}A(x,y,z)+(-1)^{d(x)d(y)}A(y,z,x)+(-1)^{d(y)d(z)}A(z,x,y)\\
=&(-1)^{d(x)d(z)}D([[x,y],z])+(-1)^{d(x)d(y)}D([[y,z],x])+(-1)^{d(y)d(z)}D([[z,x],y])\\
=&D\left((-1)^{d(x)d(z)}[[x,y],z]+(-1)^{d(x)d(y)}[[y,z],x]+(-1)^{d(y)d(z)}[[z,x],y]\right)\\
=&0.
\end{aligned}$$

Conversely, let D be a Jordan $(\theta,\varphi)_1$-prederivation of L for which (i) and (ii) hold. Then $D([[x,y],x]) = A(x,y,x)$. It follows that

$$\begin{aligned}
&D([[x+z,y],x+z]) \\
&= D([[x,y],x]) + D([[x,y],z]) + D([[z,y],x]) + D([[z,y],z]) \\
&= A(x,y,x) + A(z,y,z) + D([[x,y],z]) + D([[z,y],x])
\end{aligned}$$

and

$$\begin{aligned}
D([[x+z,y],x+z]) &= A(x+z,y,x+z) \\
&= A(x,y,x) + A(x,y,z) + A(z,y,x) + A(z,y,z).
\end{aligned}$$

Thus we obtain

$$D([[x,y],z]) + D([[z,y],x]) = A(x,y,z) + A(z,y,x). \qquad (*)$$

By (i),

$$\begin{aligned}
&A(y,x,z) \\
=&[[D(y),\theta(x)],\varphi(z)] + (-1)^{d(D)d(y)}[[\theta(y),D(x)],\varphi(z)] \\
&+ (-1)^{d(D)(d(x)+d(y))}[[\theta(y),\varphi(x)],D(z)] \\
=&-\delta(-1)^{d(x)d(y)}[[D(x),\theta(y)],\varphi(z)] - \delta(-1)^{d(x)d(y)}(-1)^{d(D)d(x)}[[\theta(x),D(y)],\varphi(z)] \\
&- \delta(-1)^{d(x)d(y)}(-1)^{d(D)(d(x)+d(y))}[[\varphi(x),\theta(y)],D(z)] \\
=&-\delta(-1)^{d(x)d(y)}[[D(x),\theta(y)],\varphi(z)] - \delta(-1)^{d(x)d(y)}(-1)^{d(D)d(x)}[[\theta(x),D(y)],\varphi(z)] \\
&- \delta(-1)^{d(x)d(y)}(-1)^{d(D)(d(x)+d(y))}[[\theta(x),\varphi(y)],D(z)] \\
=&-\delta(-1)^{d(x)d(y)}A(x,y,z).
\end{aligned}$$

This implies that

$$\begin{aligned}
D([[x,y],y]) &= -\delta(-1)^{d(x)d(y)}D([[y,x],y]) = -\delta(-1)^{d(x)d(y)}A(y,x,y) \\
&= A(x,y,y).
\end{aligned}$$

A similar argument proves

$$D([[x,y],z]) + D([[x,z],y]) = A(x,y,z) + A(x,z,y). \qquad (**)$$

By $(*)\times(-1)^{d(x)d(z)}+(**)\times(-1)^{d(x)d(y)}$, we have

$$\begin{aligned}
&(-1)^{d(x)d(z)}\big(D([[x,y],z]) + D([[z,y],x])\big)\\
&+(-1)^{d(x)d(y)}\big(D([[x,y],z]) + D([[x,z],y])\big)\\
=&(-1)^{d(x)d(z)}\big(A(x,y,z) + A(z,y,x)\big) + (-1)^{d(x)d(y)}\big(A(x,y,z) + A(x,z,y)\big),
\end{aligned}$$

then

$$\begin{aligned}
&(-1)^{d(x)d(z)}D([[x,y],z]) + (-1)^{d(x)d(y)}D([[x,y],z]) - (-1)^{d(y)d(z)}D([[y,x],z])\\
=&(-1)^{d(x)d(z)}\big(A(x,y,z) + A(z,y,x)\big) + (-1)^{d(x)d(y)}\big(A(x,y,z) + A(x,z,y)\big),
\end{aligned}$$

that is,

$$\begin{aligned}
&\Big((-1)^{d(x)d(z)} + (-1)^{d(x)d(y)} + \delta(-1)^{d(y)(d(x)+d(z))}\Big)D([[x,y],z])\\
=&\Big((-1)^{d(x)d(z)} + (-1)^{d(x)d(y)} + \delta(-1)^{d(y)(d(x)+d(z))}\Big)A(x,y,z)\\
&+(-1)^{d(x)d(z)}A(z,y,x) + (-1)^{d(x)d(y)}A(x,z,y) - \delta(-1)^{d(y)(d(x)+d(z))}A(x,y,z)\\
=&\Big((-1)^{d(x)d(z)} + (-1)^{d(x)d(y)} + \delta(-1)^{d(y)(d(x)+d(z))}\Big)A(x,y,z)\\
&+(-1)^{d(x)d(z)}A(z,y,x) + (-1)^{d(x)d(y)}A(x,z,y) + (-1)^{d(y)d(z)}A(y,x,z)\\
=&\Big((-1)^{d(x)d(z)} + (-1)^{d(x)d(y)} + \delta(-1)^{d(y)(d(x)+d(z))}\Big)A(x,y,z),
\end{aligned}$$

where the last equality uses (ii). Since ch$\mathbf{F} \neq 3$, we have $(-1)^{d(x)d(z)} + (-1)^{d(x)d(y)} + \delta(-1)^{d(y)(d(x)+d(z))} \neq 0$, and so $D([[x,y],z]) = A(x,y,z)$, i.e., D is a $(\theta,\varphi)_1$-prederivation of L.

Corollary 3.2. D is a θ-prederivation of L if and only if D is a Jordan θ-prederivation of L.

Proof. If D is a Jordan θ-prederivation of L, then (i) follows immediately. (ii) holds because

$$
\begin{aligned}
&(-1)^{d(x)d(z)}A(x,y,z)+(-1)^{d(x)d(y)}A(y,z,x)+(-1)^{d(y)d(z)}A(z,x,y)\\
=&(-1)^{d(x)d(z)}[[D(x),\theta(y)],\theta(z)]+(-1)^{d(x)d(z)}(-1)^{d(D)d(x)}[[\theta(x),D(y)],\theta(z)]\\
&+(-1)^{d(x)d(z)}(-1)^{d(D)(d(x)+d(y))}[[\theta(x),\theta(y)],D(z)]\\
&+(-1)^{d(x)d(y)}[[D(y),\theta(z)],\theta(x)]+(-1)^{d(x)d(y)}(-1)^{d(D)d(y)}[[\theta(y),D(z)],\theta(x)]\\
&+(-1)^{d(x)d(y)}(-1)^{d(D)(d(y)+d(z))}[[\theta(y),\theta(z)],D(x)]\\
&+(-1)^{d(y)d(z)}[[D(z),\theta(x)],\theta(y)]+(-1)^{d(y)d(z)}(-1)^{d(D)d(z)}[[\theta(z),D(x)],\theta(y)]\\
&+(-1)^{d(y)d(z)}(-1)^{d(D)(d(x)+d(z))}[[\theta(z),\theta(x)],D(y)]\\
=&(-1)^{d(D)d(z)}\left((-1)^{d(z)(d(D)+d(x))}[[D(x),\theta(y)],\theta(z)]\right.\\
&+(-1)^{d(y)(d(D)+d(x))}[[\theta(y),\theta(z)],D(x)]+(-1)^{d(y)d(z)}\left.[[\theta(z),D(x)],\theta(y)]\right)\\
&+(-1)^{d(D)d(x)}\left((-1)^{d(x)(d(D)+d(y))}[[D(y),\theta(z)],\theta(x)]\right.\\
&+(-1)^{d(z)(d(D)+d(y))}[[\theta(z),\theta(x)],D(y)]+(-1)^{d(x)d(z)}\left.[[\theta(x),D(y)],\theta(z)]\right)\\
&+(-1)^{d(D)d(y)}\left((-1)^{d(y)(d(D)+d(z))}[[D(z),\theta(x)],\theta(y)]\right.\\
&+(-1)^{d(x)(d(D)+d(z))}[[\theta(x),\theta(y)],D(z)]+(-1)^{d(x)d(y)}\left.[[\theta(y),D(z)],\theta(x)]\right)\\
=&0.
\end{aligned}
$$

Therefore, D is a θ-prederivation of L by Theorem 3.1.

Theorem 3.3. D is a $(\theta,\varphi)_2$-prederivation of L if and only if D is a Jordan $(\theta,\varphi)_2$-prederivation of L such that

(i) $[[D(x),\theta(y)],(\varphi-\theta)(z)]=(-1)^{d(D)d(x)}[[\theta(x),D(y)],(\varphi-\theta)(z)]$,

(ii) $(-1)^{d(x)d(z)}A'(x,y,z)+(-1)^{d(x)d(y)}A'(y,z,x)+(-1)^{d(y)d(z)}A'(z,x,y)=0$,

where $x,y,z\in L$ and $A'(x,y,z)=[[D(x),\theta(y)],\theta(z)]+(-1)^{d(D)d(x)}[[\theta(x),D(y)],\varphi(z)]+(-1)^{d(D)(d(x)+d(y))}[[\varphi(x),\varphi(y)],D(z)]$.

Proof. Let D be a $(\theta,\varphi)_2$-prederivation of L. Use the fact that

$$D([[x,y],z]) = -\delta(-1)^{d(x)d(y)}D([[y,x],z]),$$

as well as the fact that

$$\begin{aligned}
&-\delta(-1)^{d(x)d(y)}D([[y,x],z])\\
=&-\delta(-1)^{d(x)d(y)}[[D(y),\theta(x)],\theta(z)]-\delta(-1)^{d(x)d(y)}(-1)^{d(D)d(y)}[[\theta(y),D(x)],\varphi(z)]\\
&-\delta(-1)^{d(x)d(y)}(-1)^{d(D)(d(x)+d(y))}[[\varphi(y),\varphi(x)],D(z)]\\
=&[[D(x),\theta(y)],\varphi(z)]+(-1)^{d(D)d(x)}[[\theta(x),D(y)],\theta(z)]\\
&+(-1)^{d(D)(d(x)+d(y))}[[\varphi(x),\varphi(y)],D(z)],
\end{aligned}$$

then we have

$$\begin{aligned}
&[[D(x),\theta(y)],\theta(z)]+(-1)^{d(D)d(x)}[[\theta(x),D(y)],\varphi(z)]\\
=&[[D(x),\theta(y)],\varphi(z)]+(-1)^{d(D)d(x)}[[\theta(x),D(y)],\theta(z)],
\end{aligned}$$

that is, $[[D(x),\theta(y)],(\varphi-\theta)(z)] = (-1)^{d(D)d(x)}[[\theta(x),D(y)],(\varphi-\theta)(z)]$. It is routine to prove (ii).

Suppose, conversely, that D is a Jordan $(\theta,\varphi)_2$-prederivation of L satisfying (i) and (ii). Note that

$$\begin{aligned}
&A'(y,x,z)\\
=&[[D(y),\theta(x)],\theta(z)]+(-1)^{d(D)d(y)}[[\theta(y),D(x)],\varphi(z)]\\
&+(-1)^{d(D)(d(x)+d(y))}[[\varphi(y),\varphi(x)],D(z)]\\
=&-\delta(-1)^{d(x)d(y)}[[D(x),\theta(y)],\varphi(z)]-\delta(-1)^{d(x)d(y)}(-1)^{d(D)d(x)}[[\theta(x),D(y)],\theta(z)]\\
&-\delta(-1)^{d(x)d(y)}(-1)^{d(D)(d(x)+d(y))}[[\varphi(x),\varphi(y)],D(z)]\\
=&-\delta(-1)^{d(x)d(y)}[[D(x),\theta(y)],\theta(z)]-\delta(-1)^{d(x)d(y)}(-1)^{d(D)d(x)}[[\theta(x),D(y)],\varphi(z)]\\
&-\delta(-1)^{d(x)d(y)}(-1)^{d(D)(d(x)+d(y))}[[\varphi(x),\varphi(y)],D(z)]\\
=&-\delta(-1)^{d(x)d(y)}A'(x,y,z).
\end{aligned}$$

In the same way, we can get equalities (*) and (**). The rest proof is the same as the corresponding proof of Theorem 3.1.

A similar argument proves the following result.

Theorem 3.4. D is a $(\theta,\varphi)_3$-prederivation of L if and only if D is a Jordan $(\theta,\varphi)_3$-prederivation of L such that

(i) $[[D(x),(\theta-\varphi)(y)],\theta(z)] = (-1)^{d(D)d(x)}[[(\theta-\varphi)(x),D(y)],\theta(z)]$,

(ii) $(-1)^{d(x)d(z)}A''(x,y,z)+(-1)^{d(x)d(y)}A''(y,z,x)+(-1)^{d(y)d(z)}A''(z,x,y) = 0$,

where $x,y,z \in L$ and $A''(x,y,z)=[[D(x),\theta(y)],\theta(z)]+(-1)^{d(D)d(x)}[[\varphi(x),D(y)],\theta(z)] + (-1)^{d(D)(d(x)+d(y))}[[\varphi(x),\varphi(y)],D(z)]$.

Remark 3.5. Corollary 3.2 can also be concluded from Theorem 3.3 or Theorem 3.4 since for any $x,y,z \in L$, $A(x,y,z) = A'(x,y,z) = A''(x,y,z)$ when D is a Jordan θ-prederivation.

Theorem 3.6. D is a generalized $(\theta,\varphi)_1$-prederivation of L with respect to a $(\theta,\varphi)_1$-prederivation E if and only if D is a generalized Jordan $(\theta,\varphi)_1$-prederivation of L with respect to a $(\theta,\varphi)_1$-prederivation E such that

(i) $[[\theta(x),\varphi(y)],D(z)] = [[\varphi(x),\theta(y)],D(z)]$,

(ii) $(-1)^{d(x)d(z)}B(x,y,z)+(-1)^{d(x)d(y)}B(y,z,x)+(-1)^{d(y)d(z)}B(z,x,y) = 0$,

where $x,y,z \in L$ and $B(x,y,z) = [[E(x),\theta(y)],\varphi(z)]+(-1)^{d(D)d(x)}[[\theta(x),E(y)],\varphi(z)] + (-1)^{d(D)(d(x)+d(y))}[[\theta(x),\varphi(y)],D(z)]$.

Proof. Suppose that D is a generalized $(\theta,\varphi)_1$-prederivation of L with respect to a $(\theta,\varphi)_1$-prederivation E. Clearly, D is a generalized Jordan $(\theta,\varphi)_1$-prederivation of L and $D([x,y,z]) = -\delta(-1)^{d(x)d(y)}D([y,x,z])$. (i)

follows from the fact

$$\begin{aligned}
&-\delta(-1)^{d(x)d(y)}D([[y,x],z])\\
=&-\delta(-1)^{d(x)d(y)}[[E(y),\theta(x)],\varphi(z)]-\delta(-1)^{d(x)d(y)}(-1)^{d(D)d(y)}[[\theta(y),E(x)],\varphi(z)]\\
&-\delta(-1)^{d(x)d(y)}(-1)^{d(D)(d(x)+d(y))}[[\theta(y),\varphi(x)],D(z)]\\
=&[[E(x),\theta(y)],\varphi(z)]+(-1)^{d(D)d(x)}[[\theta(x),E(y)],\varphi(z)]\\
&+(-1)^{d(D)(d(x)+d(y))}[[\varphi(x),\theta(y)],D(z)].
\end{aligned}$$

Since D is a generalized $(\theta,\varphi)_1$-prederivation of L with respect to E, we have $D([[x,y],z])=B(x,y,z)$; hence

$$\begin{aligned}
&(-1)^{d(x)d(z)}B(x,y,z)+(-1)^{d(x)d(y)}B(y,z,x)+(-1)^{d(y)d(z)}B(z,x,y)\\
=&(-1)^{d(x)d(z)}D([[x,y],z])+(-1)^{d(x)d(y)}D([[y,z],x])+(-1)^{d(y)d(z)}D([[z,x],y])\\
=&D\left((-1)^{d(x)d(z)}[[x,y],z]+(-1)^{d(x)d(y)}[[y,z],x]+(-1)^{d(y)d(z)}[[z,x],y]\right)\\
=&0.
\end{aligned}$$

Conversely, if D is a generalized Jordan $(\theta,\varphi)_1$-prederivation of L with respect to a $(\theta,\varphi)_1$-prederivation E satisfying (i) and (ii), then, refer to the proof of Theorem 3.1, it suffices to prove $B(x,y,z)=-\delta(-1)^{d(x)d(y)}B(y,x,z)$. In fact,

$$\begin{aligned}
&B(y,x,z)\\
=&[[E(y),\theta(x)],\varphi(z)]+(-1)^{d(D)d(y)}[[\theta(y),E(x)],\varphi(z)]\\
&+(-1)^{d(D)(d(x)+d(y))}[[\theta(y),\varphi(x)],D(z)]\\
=&-\delta(-1)^{d(x)d(y)}[[E(x),\theta(y)],\varphi(z)]-\delta(-1)^{d(x)d(y)}(-1)^{d(D)d(x)}[[\theta(x),E(y)],\varphi(z)]\\
&-\delta(-1)^{d(x)d(y)}(-1)^{d(D)(d(x)+d(y))}[[\varphi(x),\theta(y)],D(z)]\\
=&-\delta(-1)^{d(x)d(y)}[[E(x),\theta(y)],\varphi(z)]-\delta(-1)^{d(x)d(y)}(-1)^{d(D)d(x)}[[\theta(x),E(y)],\varphi(z)]\\
&-\delta(-1)^{d(x)d(y)}(-1)^{d(D)(d(x)+d(y))}[[\theta(x),\varphi(y)],D(z)]\\
=&-\delta(-1)^{d(x)d(y)}B(x,y,z).
\end{aligned}$$

This completes the proof.

Corollary 3.7. D is a generalized θ-prederivation of L with respect to a θ-prederivation E if and only if D is a generalized Jordan θ-prederivation of L with respect to a Jordan θ-prederivation E such that

$$\begin{aligned}&(-1)^{d(z)(d(D)+d(x))}[[\theta(x),\theta(y)],(D-E)(z)]\\ &+(-1)^{d(x)(d(D)+d(y))}[[\theta(y),\theta(z)],(D-E)(x)]\\ &+(-1)^{d(y)(d(D)+d(z))}[[\theta(z),\theta(x)],(D-E)(y)]=0.\end{aligned}$$

Proof. If D is a generalized Jordan θ-prederivation of L, then (i) follows immediately. (ii) holds because

$$\begin{aligned}&(-1)^{d(x)d(z)}B(x,y,z)+(-1)^{d(x)d(y)}B(y,z,x)+(-1)^{d(y)d(z)}B(z,x,y)\\ =&(-1)^{d(x)d(z)}[[E(x),\theta(y)],\theta(z)]+(-1)^{d(x)d(z)}(-1)^{d(D)d(x)}[[\theta(x),E(y)],\theta(z)]\\ &+(-1)^{d(x)d(z)}(-1)^{d(D)(d(x)+d(y))}[[\theta(x),\theta(y)],D(z)]\\ &+(-1)^{d(x)d(y)}[[E(y),\theta(z)],\theta(x)]+(-1)^{d(x)d(y)}(-1)^{d(D)d(y)}[[\theta(y),E(z)],\theta(x)]\\ &+(-1)^{d(x)d(y)}(-1)^{d(D)(d(y)+d(z))}[[\theta(y),\theta(z)],D(x)]\\ &+(-1)^{d(y)d(z)}[[E(z),\theta(x)],\theta(y)]+(-1)^{d(y)d(z)}(-1)^{d(D)d(z)}[[\theta(z),E(x)],\theta(y)]\\ &+(-1)^{d(y)d(z)}(-1)^{d(D)(d(x)+d(z))}[[\theta(z),\theta(x)],D(y)]\\ =&(-1)^{d(x)d(z)}[[E(x),\theta(y)],\theta(z)]+(-1)^{d(x)d(z)}(-1)^{d(D)d(x)}[[\theta(x),E(y)],\theta(z)]\\ &+(-1)^{d(x)d(z)}(-1)^{d(D)(d(x)+d(y))}[[\theta(x),\theta(y)],E(z)]\\ &+(-1)^{d(x)d(y)}[[E(y),\theta(z)],\theta(x)]+(-1)^{d(x)d(y)}(-1)^{d(D)d(y)}[[\theta(y),E(z)],\theta(x)]\\ &+(-1)^{d(x)d(y)}(-1)^{d(D)(d(y)+d(z))}[[\theta(y),\theta(z)],E(x)]\\ &+(-1)^{d(y)d(z)}[[E(z),\theta(x)],\theta(y)]+(-1)^{d(y)d(z)}(-1)^{d(D)d(z)}[[\theta(z),E(x)],\theta(y)]\\ &+(-1)^{d(y)d(z)}(-1)^{d(D)(d(x)+d(z))}[[\theta(z),\theta(x)],E(y)]=\end{aligned}$$

$$
\begin{aligned}
=&(-1)^{d(D)d(z)}\big((-1)^{d(z)(d(D)+d(x))}[[E(x),\theta(y)],\theta(z)]\\
&+(-1)^{d(y)(d(D)+d(x))}[[\theta(y),\theta(z)],E(x)]+(-1)^{d(y)d(z)}[[\theta(z),E(x)],\theta(y)]\big)\\
&+(-1)^{d(D)d(x)}\big((-1)^{d(x)(d(D)+d(y))}[[E(y),\theta(z)],\theta(x)]\\
&+(-1)^{d(z)(d(D)+d(y))}[[\theta(z),\theta(x)],E(y)]+(-1)^{d(x)d(z)}[[\theta(x),E(y)],\theta(z)]\big)\\
&+(-1)^{d(D)d(y)}\big((-1)^{d(y)(d(D)+d(z))}[[E(z),\theta(x)],\theta(y)]\\
&+(-1)^{d(x)(d(D)+d(z))}[[\theta(x),\theta(y)],E(z)]+(-1)^{d(x)d(y)}[[\theta(y),E(z)],\theta(x)]\big)\\
=&0.
\end{aligned}
$$

Note that E is a θ-prederivation by Corollary 3.2. Therefore, D is a generalized θ-prederivation of L with respect to a θ-prederivation E by Theorem 3.6.

As before, one can prove the following theorems.

Theorem 3.8. D is a generalized $(\theta,\varphi)_2$-prederivation of L with respect to a $(\theta,\varphi)_2$-prederivation E if and only if D is a generalized Jordan $(\theta,\varphi)_2$-prederivation of L with respect to a $(\theta,\varphi)_2$-prederivation E such that

(i) $[[E(x),\theta(y)],(\varphi-\theta)(z)]=(-1)^{d(D)d(x)}[[\theta(x),E(y)],(\varphi-\theta)(z)]$,

(ii) $(-1)^{d(x)d(z)}B'(x,y,z)+(-1)^{d(x)d(y)}B'(y,z,x)+(-1)^{d(y)d(z)}B'(z,x,y)=0$,

where $x,y,z\in L$ and $B'(x,y,z)=[[E(x),\theta(y)],\theta(z)]+(-1)^{d(D)d(x)}[[\theta(x),E(y)],\varphi(z)]+(-1)^{d(D)(d(x)+d(y))}[[\varphi(x),\varphi(y)],D(z)]$.

Theorem 3.9. D is a generalized $(\theta,\varphi)_3$-prederivation of L with respect to a $(\theta,\varphi)_3$-prederivation E if and only if D is a generalized Jordan $(\theta,\varphi)_3$-prederivation of L with respect to a $(\theta,\varphi)_3$-prederivation E such that

(i) $[[E(x),(\theta-\varphi)(y)],\theta(z)]=(-1)^{d(D)d(x)}[[(\theta-\varphi)(x),E(y)],\theta(z)]$,

(ii) $(-1)^{d(x)d(z)}B''(x,y,z)+(-1)^{d(x)d(y)}B''(y,z,x)+(-1)^{d(y)d(z)}B''(z,x,y)=0$,

where $x, y, z \in L$ and $B''(x,y,z) = [[E(x), \theta(y)], \theta(z)] + (-1)^{d(E)d(x)}[[\varphi(x), E(y)], \theta(z)] + (-1)^{d(D)(d(x)+d(y))}[[\varphi(x), \varphi(y)], D(z)]$.

Remark 3.10. Corollary 3.7 can also be concluded from Theorem 3.8 or Theorem 3.9, since for any $x, y, z \in L$, $B(x,y,z) = B'(x,y,z) = B''(x,y,z)$ when D is a generalized Jordan θ-prederivation.

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HADRONIC CHEMISTRY AND BINDING ENERGIES[1]

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Abstract

In this paper we have reviewed in some what considerable details the valence bond treatment based on the proposal of *isoelectronium* by Santilli and his iso-mathematics. It is now known as hadronic chemistry. We have discussed the cases of hydrogen, water and magnecules with the emphasis on their energetics. We have taken this opportunity also to re-examine Eyring's transition state theory based assertion of a shallow minima at the top of the barrier for bimolecular chemical reactions by juxtaposing the *isoelectronium* of two electrons in a singlet state to the requirement of three electron bonding of the activated complex. The answer obtained is in negation that is there is no possibility of achieving any stability of activated complex even by marginal amount.

Keywords: Hadronic chemistry, Isomathematics, Quantum chemistry, Chemical kinetics.

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1 Introduction

The quantum mechanical calculations of energies of simple atoms and molecules by different methods and techniques are being extensively undertaken since past more than 50 years. The quantum mechanical results of calculations of binding energies of neutral molecules by different methods have always fascinated chemists and physicists across the globe. The most commonly used are the variation and perturbation methods [1–3]. The perturbation method uses the solution for energy of zero order systems to find a solution for the required system in hand. Whereas, the variation method consists of Linear Combination of Atomic Orbitals (LCAO) to generate Molecular Orbitals (MO). Hence it is also referred as LCAO-MO theory or in short MO theory. Other notable variant of variation method is the Self-consistent Field (SCF) theory. These variation methods involve approximations and as a result of this the binding energies so obtained do not accurately match with the experimental values [1, 2]. The energy calculated for H_2 molecule by LCAO-MO method is observed to be -1.0985 a.u. (Binding energy = - 2.681 eV) as against the experimental value of -1.174 a.u. (Binding energy = - 4.75 eV). By applying the valence-bond (VB) theory (Hitler-London) [1–3] the value for energy is observed to be -1.1160 a.u. (Binding energy =-3.140 eV). Thus apparently it is observed that the VB method is better than MO theory but this conclusion is not justified as both are gross approximations to the actual state of affairs in the molecule. One of the great shortcomings of the MO theory is that the ionic terms enter into the wave function with the same weight as nonionic terms. This structuring is generally overcome by arbitrarily introducing weightage factors to suit calculations. In VB theory the wave function consists of the covalent part only. Thus, one is tempted to conclude that it is perhaps better to leave altogether the ionic terms out of the wave functions for Hydrogen molecule.

The primary structural characteristics of quantum chemistry are,

1. Linearity, Eigen value equations depend upon wave functions only to the first power.

2. Local- differential, in the sense of acting among a finite number of

isolated points; and

3. Potential, in the sense that all acting forces are derivable from a potential field.

Thus quantum theory is a Hamiltonian theory i.e. models are completely characterized by the sole knowledge of the Hamiltonian operator, with unitary structure:

$$U = e^{iH \times t}, \quad U \times U^{\dagger} = U^{\dagger} \times U = I, \quad H = H^{\dagger} \tag{1}$$

20^{th} century was dominated by achievements in quantum chemistry. It has helped to solve even very complicated problems. It has been a basis for the evolution of molecular spectroscopy. The spectroscopy could explain several phenomena related with the complex structure of molecules. Despite these achievements quantum chemistry cannot be considered as an unambiguous tool because there are of several insufficiencies in it.

One of the most important insufficiencies is the inability to represent deep mutual penetrations of the wavepackets of valence electrons in molecular bonds. This is so because two electrons in the same molecular orbital should experience a strong repulsion. But in reality the valence electrons of two atoms form a strong and stable union that can happen if and only if a very strong attraction between two electrons of a molecular orbital exists overcoming their electrostatic repulsion. The latter interaction is known to be,

1. Nonlinear, i.e. dependent on powers of the wavefunctions grater than one;

2. Non-integral, i.e. dependent on integrals over the volume of overlapping, which as such, cannot be reduced to a finite set of isolated points; and

3. Nonpotential, i.e., consisting of "contact" interactions with consequential "zero range" for which the notion of potential energy has no mathematical or physical sense.

This requires a non-Hamiltonian theory, that is a theory which cannot be solely characterized by Hamiltonian, based on a new nonunitary law [4]:

$$U \times U^{\dagger} = U^{\dagger} \times U \neq I \tag{2}$$

The above law is formulated on conventional Hilbert spaces over conventional fields.

Thus above features are beyond any hope of scientific quantitative treatment via quantum mechanics and chemistry.

In the light of above facts Professor Santilli opined that the fundamental quantum chemical notion of valence bond as presented in the 20th century literature is pure nomenclature without any quantitative scientific content because to be quantitative the preceding notion should,

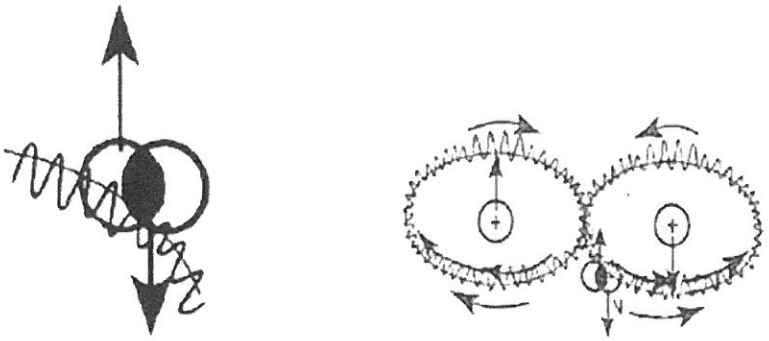
1. identify clearly the force between two identical valence electrons,

2. prove that such a force is attractive as an evident necessary prerequisite to claim the sufficiently strong bond needed for molecule formation, and

3. prove that such a clearly identified and clearly attractive force verifies indeed the experimental data on molecular structures.

Thus, it is impossible for quantum chemistry to meet the above conditions because in quantum mechanics one uses the Coulomb law to describe the interactions between two identical electrons that obviously maintain that the two identical electrons must repel each other and certainly they cannot attract each other. Santilli never accepted these notions of so-called well established theory of quantum chemistry. His untiring efforts of a few decades gave birth to the new discipline of Hadronic Chemistry [4]. Hadronic chemistry of small molecules is based on Santilli's iso- and genomathematics by considering the interactions at 10^{-15}m or less [4–6]. The main idea is that at such short distances the wavepackets of electrons lose their point like character considered at atomic distances rather they overlap each other considerably (see Figure 1).

Molecular structures are considered as isolated, thus being closed, conservative and reversible, the applicable branch of hadronic chemistry is isochemistry. It is characterized by the identification of the nonunitary time



(a) (b)

Figure 1: (a) In the left Figure: Schematic representation of the deep overlapping of the wavepackets of the valence electrons in singlet coupling (that meets the Pauli exclusion principle). These conditions are known to be nonlinear, nonlocal and nonpotential (due to the zero-range contact interactions) is shown, thus not possible to be represented via Hamiltonian and consequently not being unitary. As a result, the ultimate nature of the valence bonds is outside any credible representation via quantum chemistry. The Hadronic Chemistry has been built for the specific scope of representing the conditions considered herein of the bonding valence electrons. (b) In the right Figure: Schematic representation of Isochemical model of Hydrogen Molecule showing oo shaped orbit of isoelectronium.

evolution with generalized unit of theory, called isounit,

$$U \times U^\dagger = U^\dagger \times U = \hat{I}(r,\, p,\, \psi,\, \partial\psi, \cdots\cdots) \neq I \tag{3}$$

The isounit can represent nonlinear nonlocal and nonhamiltonian interactions. On the other hand, quantum mechanics and chemistry are valid at all the distances of the order of the Bohr radius ($\approx 10^{-8}$cm), and the covering hadronic chemistry holds at distance of the order of size of the wavepackets of valence electrons ($\approx 10^{-13}$cm).

The above condition is achieved by imposing that all isounits recover the conventional unit at a distance grater than 1fm.

$$\lim_{r \geq 1fm} \hat{I}(r,\, p,\, \psi,\, \partial\psi, \cdots\cdots) = I \tag{4}$$

and for $r \leq 1fm$

$$\hat{I} \gg 1,\ \widehat{T} \ll 1 \tag{5}$$

Thus, under the condition $r \geq 1fm$, hadronic chemistry recovers quantum chemistry. The conditions given in Equations (4) and (5) are verified by actual chemical models. Quantum mechanics has been able to achieve an exact representation of all experimental data for structure of a single hydrogen atom and hydrogen like atoms. Therefore quantum mechanics is assumed to be exactly valid within such a well defined physical system.

However, quantum mechanics and chemistry have not been able to achieve an exact representation of experimental data on molecular structures, where conditions are entirely different. As a result, these theories cannot be considered as being exactly valid for different conditions of molecular bonds. It has been proved that hadronic chemistry provides an exact representation of molecular characteristics.

The present study is aimed at reviewing energetics of H_2, H_2O and a representative magnecular species using the methods of Hadronic Chemistry. Recently Tangde has reviewed to some extent the subject matter of hadronic chemistry of hydrogen and water molecules lucidly [7].

2 Background Behind Hadronic Chemistry of Covalent Bond

For the sake of brevity we are describing only two major aspects, one that leads us to the concept of isoelectronium and the other one describes incapability of quantum chemistry to establish why a covalent bond is formed between only two atoms and not three or more atoms. The details of the following aspects and allied ones have been described in references [4–6] by Santilli himself.

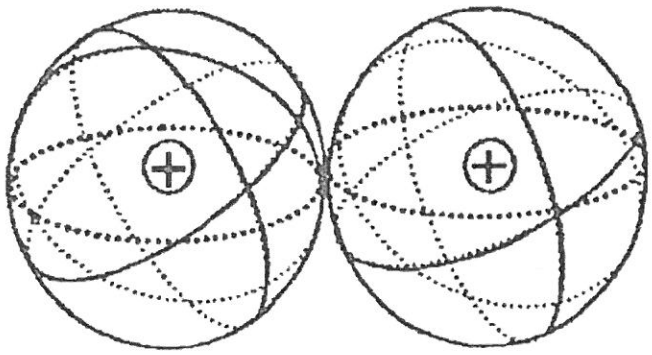


Figure 2: A schematic view of the contemporary physical (and not chemical)conception of the simplest posible molecule, the hydrogen molecule, at absolute zero degree temperature, herein conceptually represented as two H-atoms next to each other in the absence of any rotation and vibration motion. Therefore, the spheres represent the spherical distribution of the orbits (and not the orbitals) of the individual electrons.

2.1 Quantum Chemistry Description of a Covalent Bond Lacks Sufficiently Strong Binding Force

It is well known that the Coulomb forces between electrons and nucleons of an atom remain completely balanced. That is there remain no residual Coulomb forces as atoms are electrically neutral. Thus for forming a molecule from atoms there exists no Coulomb attractive force at all. As a result of this the union, say between two hydrogen atoms, would look like the one depicted in Figure 2, That is the individual electron would have spherical distribution of its orbits about its nucleus. More quantitative description of the state of affairs gets lucidly explained using following diagram (Figure 3):

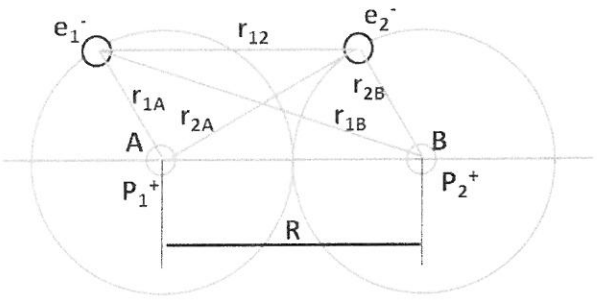


Figure 3: A schematic view of the fact that the total Coulomb force among two atoms of a molecular structure is identically null in the semiclassical approach. As a consequence, the conventional Coulomb interactions cannot be a credible ground for molecular bonds.

where in Figure 3 e_1^- and e_2^- are two electrons, A and B are two protons of separate atoms, r_{12} is the distance between electrons, R is distance between two protons, r_{1A}, r_{2B}, r_{1B} and r_{2A} are the self explanatory distances.

Using the diagram of Figure 3 it is easy to demonstrate that the sum of the two cross attractive forces between electrons and protons get exactly compensated by the sum of the repulsive forces between electron-electron and proton-proton. Hence there remains no attractive force between two hydrogen atoms. This gets quantitatively demonstrated using corresponding Schrödinger wave equation of quantum chemistry, namely:

$$\left(\frac{p_1^2}{2\mu_1}+\frac{p_2^2}{2\mu_2}-\frac{e^2}{r_{1A}}-\frac{e^2}{r_{2A}}-\frac{e^2}{r_{1B}}-\frac{e^2}{r_{2B}}+\frac{e^2}{r_{12}}+\frac{e^2}{R}\right)\times|\psi\rangle = E\times|\psi\rangle \quad (6)$$

where, μ_1 and μ_2 are the reduced masses of electrons, 1 and 2, and p_1 and p_2 are the linear momentum operators of two electrons. Notice that in writing equation (6) the protons have been assumed at rest.

Now as described above the potential energy terms involving r_{1B}, r_{2A}, R and r_{12} get nullified amongst themselves. Therefore equation (6) reduces to,

$$\left[\left(\frac{p_1^2}{2\mu_1}-\frac{e^2}{r_{1A}}\right)+\left(\frac{p_2^2}{2\mu_2}-\frac{e^2}{r_{2B}}\right)\right]\times|\psi\rangle = E\times|\psi\rangle \quad (7)$$

Notice that the terms leftover are kinetic energy of two electrons and potential enery of attraction of two electrons with their respective protons. Thus equation (7) does not involve distance between two nuclei and at what distance the two hydrogen atoms are considered in this equation is not known. But the solution of equation (7) would produce the sum of binding energies of two electrons with their respective protons in forming atoms and not the binding energy of the hydrogen molecule. Also notice that equation (7) does not have any term describing interaction between two electrons attractive or repulsive one. Hence it does not mean that the two atoms considered by equation (7) are bonded. But for bonding of hydrogen atoms to occur there must be an attractive force between two atoms and we need to introduce corresponding term in equation (7). As the hydrogen molecule and for that matter all molecules are stable unions that shows that there exists an attractive force leading to bond formation. To quantify this attractive force Santilli proposed the concept of isoelectronium formed by strong overlap of wavepackets of two electrons and that results in the operation of Hulthén potential below the distances of 1fm that produces a very strong attractive force. On introducing this attractive term in equation (7) we obtain the correct Schrödinger wave equation, that reads as,

$$\left[\left(\frac{p_1^2}{2\mu_1}-\frac{e^2}{r_{1A}}\right)+\left(\frac{p_2^2}{2\mu_2}-\frac{e^2}{r_{2B}}\right)-V'\frac{e^{-b\times r_{12}}}{1-e^{-b\times r_{12}}}\right]\times|\psi\rangle=E'\times|\psi\rangle \quad (8)$$

Notice that in equation (8) now there appears E' instead of E this is so because a new Hulthén term appears in it. However, the arriving at equation (8) described above is simplistic way to accommodate the overall attractive force in forming an *isoelectronium.*

2.2 Incapability of Quantum Chemistry to Explain Why a Chemical Bond is Formed Between Two Atoms Only

In quantum chemistry for hydrogen molecule one uses equation (6) but as stated above it reduces effectively to equation (7). On the same lines three or more hydrogen atoms can form a molecular union according to quantum chemistry as depicted in Figure (4) for a representative H_3 molecule.

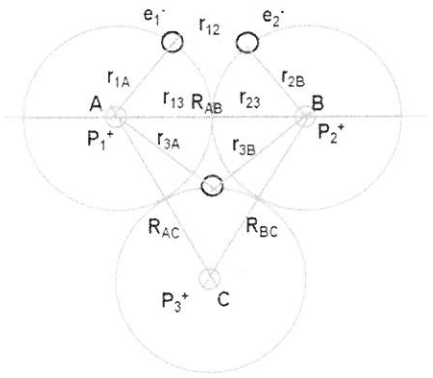


Figure 4: A schematic view of the fact that the current conception of the structure of hydrogen molecule admits a third hydrogen atom, with molecular structure H_3 and consequently, an arbitrary number of H-atoms, thus admitting molecules of generic type H_5, H_{27} etc. Herein it is being depicted that the structure H_3 if conceived as a molecule then it should also admit H_4, H_5 etc., which have been never detected.

It can be shown that all cross attractive terms get exactly compensated by repulsive terms amongst the protons as well as amongst electrons in the Schrödinger equation of quantum chemistry. Because of unawareness of it quantum chemistry appears to allow 2 or more atoms to form a molecular union. Hence it is concluded by Santilli that the quantum chemistry is incapable of answering the observation that why there are only two hydrogen atoms in the hydrogen as well as in water molecules.

3 Concept of Isoelectronium

R. M. Santilli and D. D. Shillady have developed the conceptual foundations of their isochemical model of molecular bonds for H_2 molecule [8]. It was assumed that pairs of valence electrons from two different atoms can bond themselves at short distances into a singlet quasi-particle state called "isoelectronium" which describes an oo-shaped orbit around the individual

H atom. It is shown in Figure 5 given below.

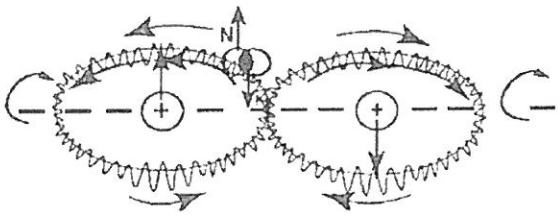


Figure 5: A schematic representation of isoelectronium orbiting in the oo-shaped orbit about two proptons of hydrogen molecule.

The primary binding force of the isoelectronium is assumed to be of nonlinear, nonlocal, and nonpotential type due to contact effects in deep overlapping of the wavepackets of valence electrons. The isoelectronium is expected to have a component of the binding force of purely potential type because when the electrons are in singlet coupling, the magnetostatic attraction may considerably bigger than the electrostatic repulsion at distances of one Fermi or less (see Figure 6),

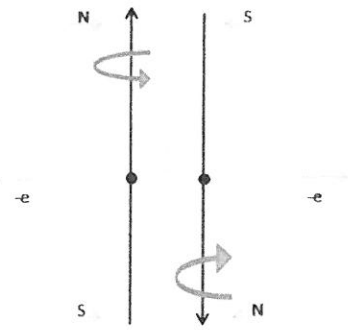


Figure 6: A schematic representation of the origin of force of magnetostatic attraction between two electrons in a singlet coupling which overwhelmingly overcomes the electrostatic repulsion between them.

Figure 6 explains conventional coulomb forces of electrostatic and magnetostaic type in the structure of electronium. Since the charges are equal, they cause repulsion. However, since the coupling is in singlet, the magnetic polarities are opposite, thus implying an attraction. The calculations by Santilli have shown that magnetostatic attractions are equal to the electrostastic repulsions at a mutual distance of the order of 1fm, while it becomes bigger at smaller distances. This is the reason why hadronic horizon has been set at 10^{-13}cm. Thus bonding force of isoelectronium can see its origin on purely columbic forces and, more particular on the dominance of magnetic over electric effects at short distances. However, isoelectronium cannot be treated with in purely quantum mechanical context for various reasons. The first reason is that with the decrease of the distance, both electrostatic and magnetic effects diverge. This prevents any serious scientific study. Hadronic mechanics and chemistry have been built precisely to remove these divergences via isotopies of generic products:

$$A\widehat{\times}B = A \times \widehat{T} \times B \qquad \text{with} \qquad |\,\widehat{T}\,| \ll 1 \tag{9}$$

Therefore, the hadronic treatment of isoelectronium permits convergent numerical predictions which would be otherwise impossible for quantum chemistry.

4 Santilli and Shillady Model of Hydrogen Molecule

4.1 Santilli-Shillady strong valence bond

Santilli and Shillady in a novel paper of 1999 developed a new concept of strong valence bond [8]. Their development we describe below stepwise.

Recall that that the isoelectronium consists of two electrons in singlet coupling shown in Figure 7.

Now let us apply the conventional quantum chemistry to free isoelectronium. Herein we need to consider kinetic energy and electrostatic repulsion amongst two electrons of isoelectronium. The velocity and mass of both

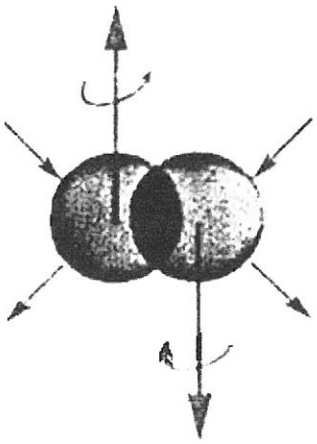


Figure 7: A schematic representation of isoelectronium with deep overlaping of the wavepackets of two electrons in singlet coupling.

the electrons of isoelectronium would be identically same and hence the Schrödinger wave equation would read as,

$$\left(\frac{p^2}{m} + \frac{e^2}{r}\right) \times |\psi\rangle = E \times |\psi\rangle \tag{10}$$

where, r is the distance between two electrons of isoelectronium and m is the mass of electron. The above equation shows the repulsive Coulomb force between the point-like charges of the electrons. But as stated above the electrons have extended wavepackets of the order of 1 fm whose mutual penetration, as necessary for the valence bond formation, causes nonlinear, nonlocal and nonpotential interactions that constitute the foundations of hadronic mechanics. The only known possibility for an invariant representation of these interactions is to exit from the class of unitary equivalence of equation (10) via an isounitary transformation.

Note that equation (10) still does not admit the attractive forces between the pair of singlet electrons and is not bound to any nuclei. These two aspects have been well attended by introducing conventional nonunitary

form that reads as,

$$0 < U \times U^{\dagger} = U^{\dagger} \times U = \hat{I} = \frac{1}{\widehat{\widehat{T}}} \neq I \tag{11}$$

Also notice that through a simple mathematical manipulation we have the following transformation,

$$\hat{p} \times \widehat{T} \times \hat{p} \times \widehat{T} = p \times \hat{I} \times \widehat{T} \times p \times \hat{I} \times \widehat{T} = p^2 \tag{12}$$

Hence equation (10) transforms to,

$$\left(\frac{\hat{p} \times \widehat{T} \times \hat{p} \times \widehat{T}}{m} + \frac{e^2}{r} \right) \times \widehat{T} \times |\hat{\psi}\rangle = E \times |\hat{\psi}\rangle \tag{13}$$

or

$$\left(\frac{\hat{p} \times \widehat{T} \times \hat{p} \times \widehat{T}}{m'} + \frac{e^2}{r} \times \widehat{T} \right) \times |\hat{\psi}\rangle = E \times |\hat{\psi}\rangle \tag{14}$$

where m' is the isomass of electron. Notice that the electronic term is now supposed to take care of the repulsive as well as attractive forces between the pair of electrons forming isoelectronium. Still equation (14) has not admitted another requirement for a stable isoelectronium that is bounded to an atom. Hence we need to externally add the corresponding term in equation (14). Let us consider generalized case of nucleus with positive charge Ze. By incorporating this fact equation (14) transforms to,

$$\left(\frac{\hat{p} \times \widehat{T} \times \hat{p} \times \widehat{T}}{m'} + \frac{e^2}{r} \times \widehat{T} - \frac{Ze^2}{R} \right) \times |\hat{\psi}\rangle = E' \times |\hat{\psi}\rangle \tag{15}$$

Notice again that we have E' instead of E in equation (14) for the obvious reasons.

Santilli and Shillady introduced the following realization of the nonunitory transform, that is, of the *fundamental isounit of hadronic chemistry.*

$$\begin{aligned} U \times U^{\dagger} = \hat{I} = \frac{1}{\widehat{\widehat{T}}} &= \exp\left(\left[\psi(r)/\hat{\psi}(r) \right] \int \psi^{\dagger}_{1\downarrow}(r) \times \psi_{2\uparrow} d^3 r \right) \\ &= 1 + \left[\psi(r)/\hat{\psi}(r) \right] \int \psi^{\dagger}_{1\downarrow}(r) \times \psi_{2\uparrow} d^3 r + \cdots\cdots \end{aligned} \tag{16}$$

where ψ and $\hat{\psi}$ are the solutions using unitary and non-unitory equations respectively and ψ_k , $k = 1, 2, ..$ are the conventional quantum mechanical wave functions of the two electrons.

The above isounit represents interactions that are nonlinear, non-local and nonpotential. Additionally, for all mutual distances between the valence electrons greater than 1 fm, the volume integral of equation (16) is null with limit:

$$\lim_{r>1fm} = 1 \tag{17}$$

under that hadronic chemistry recovers quantum chemistry identically and uniquely.

Now let us consider the expression of $\hat{I}$ and $\widehat{T}$ to the first approximation [9–11].

$$\hat{I} = e^{N\times\psi/\hat{\psi}} \approx 1 + N \times \frac{\psi}{\hat{\psi}}, \qquad N = \int \psi^{\dagger}_{1\downarrow}(r) \times \psi_{2\uparrow}(r)\, d^3r \tag{18}$$

and we have

$$\widehat{T} \approx 1 - N \times \frac{\psi}{\hat{\psi}} \tag{19}$$

and

$$| \hat{I} | \gg 1, \quad | \widehat{T} | \ll 1, \quad \lim_{r\gg 1fm} \widehat{I} = I \tag{20}$$

As the explicit form of ψ is of Coulomb type, it behaves as,

$$\psi(r) \approx N \times e^{-(b\times r)} \tag{21}$$

where N is approximately constant at distances near the hadronic horizon of radius,

$$r_c = \frac{1}{b} \tag{22}$$

while $\hat{\psi}$ behaves like,

$$\hat{\psi} \approx M \times \left(\frac{1 - e^{-(b\times r)}}{r} \right) \tag{23}$$

where M is also approximately constant within the same range of applicability [4], then we have

$$\widehat{T} \approx 1 - \frac{N^2}{M} \times \frac{e^{-(b\times r)}}{1 - e^{-(b\times r)}} \times r = 1 - V_0 \frac{e^{-(b\times r)}}{1 - e^{-(b\times r)}} = \left(1 - \frac{V_{Hulthén}}{r}\right) \quad (24)$$

where

$$V_{Hulthén} = V_0 \times \frac{e^{-(b\times r)}}{1 - e^{-(b\times r)}} \times r, \quad V_0 = \left(\frac{N^2}{M} \times r\right) \quad (25)$$

In this way there appeared the *attractive Hulthén potential*, $V_{Hulthén}$, in our mathematical quantitative description. However, the Hulthén potential is known to behave like the Coulomb potential at short distances and is much stronger than the latter one. Thus on assuming $N \approx M$ we obtain,

$$\frac{V_{Hulthén}}{r} \approx \frac{V_0}{b} \times \frac{1}{r} = \frac{N}{b} = \frac{1}{b} \quad \text{as} \quad N \to 1 \quad (26)$$

Hence, inside the hadronic horizon we can ignore repulsive (attractive) conventional Coulomb forces altogether and can write the Coulomb term of equation (15) as,

$$\begin{aligned} +\frac{e^2}{r} \times \widehat{T} - \frac{Z \times e^2}{R} \quad &\approx \quad \frac{e^2}{r} \times \left(1 - \frac{V_{Hulthén}}{r}\right) - \frac{Z \times e^2}{R} \\ &= -V' \times \frac{e^{-(b\times r)}}{1 - e^{-(b\times r)}} \end{aligned} \quad (27)$$

where the use of a new constant in preceding equation reflects the "absorption" of the repulsive Coulomb potential by the much stronger attractive Hulthén potential.

In this way Santilli and Shilliady have achieved the strong valence bond for the first time in the history of chemistry namely a valence coupling between two identical electrons in the singlet coupling with strong attractive force.

Therefore, equation (15), an iso-Schrödinger equation, reads as,

$$\left(\frac{\hat{p} \times \widehat{T} \times \hat{p} \times \widehat{T}}{m'} - V' \times \frac{e^{-(b\times r)}}{1 - e^{-(b\times r)}}\right) \times |\hat{\psi}\rangle = E' \times |\hat{\psi}\rangle \quad (28)$$

Notice that all Columbic terms have been absorbed, that has generated Hulthén term in equation (28). Of course, we are at will to absorb all or some of the coulomb terms and hence the value and nature of corresponding V' will be different in each case.

By assuming in the first approximation $\widehat{T} = \rho \approx 1$ the radial equation of the model reduces to the model of π^0 meson [10] or of the Cooper pair [11] although with different values of V and b. Thus we have,

$$\left[\frac{1}{r^2}\left(\frac{d}{dr}r^2\frac{d}{dr}\right) + \frac{m}{\rho^2 \times \hbar^2} \times \left(E' + V' \times \frac{e^{-(b\times r)}}{1 - e^{-(b\times r)}}\right)\right] \times |\hat{\psi}\rangle = E' \times |\hat{\psi}\rangle \quad (29)$$

The exact solution with related boundary conditions was first computed by Animalu [10] and remain fully applicable to isoelectronium. The resulting spectrum is Hulthén potential. The solution of equation (29) is,

$$\mid E' \mid = \frac{\rho^2 \times \hbar^2 \times b^2}{4 \times m}\left(\frac{m \times V}{\rho^2 \times \hbar^2 \times b^2} \times \frac{1}{n} - n\right)^2 \quad (30)$$

and it possesses a finite spectrum.

Now on introducing the parametrization,

$$k_1 = \frac{1}{\lambda \times b} \quad \text{and} \quad k_2 = \frac{m \times V}{\rho^2 \times \hbar^2 \times b^2} \quad (31)$$

Further, under first nonrelativistic approximation, namely:

$$k_2 = \frac{m \times V}{\rho^2 \times \hbar^2 \times b^2} = 1 \quad (32)$$

and by assuming that V is of the order of the magnitude of the total energy of the isoelectronium at rest [9–11], we have,

$$V \approx 2 \times \hbar \times \omega = 2 \times 0.5\text{MeV} = 1\text{MeV} \quad (33)$$

Now for $\rho = 1$ we have,

$$\begin{aligned} r_c = b^{-1} &\approx \left(\frac{\hbar^2}{m \times V}\right)^{1/2} \\ &= \left(\frac{\hbar}{m \times \omega_0}\right)^{1/2} = \left(\frac{1.054 \times 10^{-27}\text{erg.s}}{1.82 \times 10^{-27}\text{g} \times 1.236 \times 10^{20}\text{Hz}}\right) \\ &= 6.8432329 \times 10^{-11} cm = 0.006843\text{A}^0 \end{aligned} \quad (34)$$

The actual radius of the isoelectronium, when considered to be a quasi-particle is expected to vary with trigger i.e. with the nuclear charges. This illustrates the upper boundary characteristic values of V and r_c.

The value of k_1 is then given by,

$$k_1 = \frac{V}{2 \times k_2 \times b \times c_0} = 0.19, \quad k_2 \approx 1 \tag{35}$$

The above two values for isoelectronium are quite close to the corresponding values of π^0 [10] and the Cooper pair [11].

It should be noted that at this nonrelativistic approximation, the binding energy of the isoelectronium is not only unique but also identically null,

$$\mid E_0 \mid = \frac{\rho^2 \times \hbar^2 \times b^2}{4 \times m} \left(\frac{m \times V}{\rho^2 \times \hbar^2 \times b^2} \times -1 \right)^2 = \frac{V}{4 \times k_2} \times (k_2 - 1)^2 = 0 \tag{36}$$

This result is crucial to prevent inconsistencies with Pauli's exclusion principle, which requires no potential energy between the two electrons for its interpretation in a way consistent with experimental data.

Thus, the lack of binding energy of the isoelectronium is the most important information. In fact, it transfers the representation of the binding energy of molecular bonds to the motion of the isoelectronium in a molecular structure. A novelty of isochemistry over quantum chemistry is that the mutual distance (charge diameter) between the two isoelectrons in the isoelectronium could, as a limiting case, also be identically null, that is two isoelectrons could be superimposed in a singlet state. This limit case is intriguing because it yields the value $-2e$ for charge of isoelectronium, the null value of the relative kinetic energy and identical null magnetic field. This is perfectly a diamagnetic state, which evidently allows a better stability of the isochemical bond as compared to a quasi-particle with non-null size.

It is worth noting here that, under the transform (equation (18)), model (equation (21)) is implemented with interactions which are nonlinear, due to the factor $\psi/\hat{\psi}$ in the exponent; nonlocal, because of the volume integral in equation (18) and nonpotential, because not represented by a Hamiltonian. The explicit form of the isotopic element $\widehat{T}$, equation (19), emerges in a

rather natural way as being smaller than one in absolute value, equation (20); i.e.,

$$\mid \widehat{T} \mid = \mid 1 - N \times (\psi/\hat{\psi}) \mid \ll 1 \tag{37}$$

This property alone is sufficient to guarantee that all slowly convergent series of quantum chemistry converge faster in the domain of isochemistry.

4.2 Isochemical model of hydrogen molecule with stable isoelectronium

4.2.1 A four-body isochemical model

Santilli and Shillady developed the isochemical model for the hydrogen molecule [8] by identifying the equation of structure of the hydrogen molecule under limit assumption that the isoelectronium is stable at short distances, namely, that the two valence electrons are permanently trapped inside the hadronic horizon.

From preceding Subsection we have,

$$\begin{aligned} \text{mass} &= 1\text{MeV},\ \text{Spin} = 0,\ \text{Charge} = 2 \times e,\ \text{Magnetic moment} \approx 0 \\ \text{radius} &= r_c = b^{-1} = 6.8432329 \times 10^{-11}\text{cm} = 0.006843\text{A}^0 \end{aligned}$$

Considering the conventional quantum model of H_2 molecule (as shown in Figure 3) one writes,

$$\left(\frac{1}{2\mu_1} p_1 \times p_1 + \frac{1}{2\mu_2} p_2 \times p_2 + \frac{e^2}{r_{12}} - \frac{e^2}{r_{1A}} - \frac{e^2}{r_{2A}} - \frac{e^2}{r_{1B}} - \frac{e^2}{r_{2B}} + \frac{e^2}{R}\right) \times \mid \psi\rangle = E \times \mid \psi\rangle \tag{38}$$

where 1, 2 represent the two electrons; a, b represent the two protons; and R is the distance between the protons as shown in Figure 3.

Now on subjecting the above model to the transform,

$$U \times U^\dagger \mid_{r \approx r_c} = \hat{I} = \frac{1}{\widehat{T}} \neq I \tag{39}$$

which is nonunitary only at short mutual distances,

$$\text{radius} = r_c = b^{-1} = r_{12} = 6.8432329 \times 10^{-11}\text{cm} \tag{40}$$

and becomes unitary at larger distances,

$$U \times U^{\dagger} \mid_{r \leq 10^{-10}\text{cm}} \neq I, \quad I_{r \gg 10^{-10}\text{cm}} = I \tag{41}$$

It is easy to realize that the nonunitary transform shall act only on the r_{12} variable leaving all others unchanged, so Santilli and Shillady adopted,

$$U(r_{12}) \times U^{\dagger}(r_{12}) = \hat{I} = \exp\left[\frac{\psi(r_{12})}{\hat{\psi}(r_{12})} \int d^3 r_{12} \hat{\psi}^{\dagger}{}_{1\downarrow}(r_{12}) \times \hat{\psi}_{2\uparrow}(r_{12})\right], \tag{42}$$

where ψ and $\hat{\psi}$ are the conventional and isowavefunctions respectively.

The isounitary transform of equation (38) showing the short range terms (isochemistry) and simple addition of long range terms (quantum chemistry) yields the radial equation as,

$$\left(-\frac{\hbar^2}{2 \times \mu_1}\widehat{T} \times \nabla_1 \times \widehat{T} \times \nabla_1 - \frac{\hbar^2}{2 \times \mu_2}\widehat{T} \times \nabla_2 \times \widehat{T} \times \nabla_2 + \frac{e^2}{r_{12}} \times \widehat{T} - \frac{e^2}{r_{1A}} - \frac{e^2}{r_{2A}} - \frac{e^2}{r_{1B}} - \frac{e^2}{r_{2B}} + \frac{e^2}{R}\right) \times \mid \hat{\psi}\rangle = E \times \mid \hat{\psi}\rangle \tag{43}$$

As Hulthén potential behaves like the Coulomb one at small distances, equation (43), on absorbing all Coulomb terms of interactions becomes,

$$\left(-\frac{\hbar^2}{2 \times \mu_1} \times \nabla_1^2 - \frac{\hbar^2}{2 \times \mu_2} \times \nabla_2^2 - V' \times \frac{e^{-r_{12} \times b}}{1 - e^{-r_{12} \times b}}\right) \times \mid \hat{\psi}\rangle = E \times \mid \hat{\psi}\rangle \tag{44}$$

which can also be written as,

$$\left(\frac{p_{isoelec}^2}{2 \times m_{isoelec}} - V' \times \frac{e^{-r \times b}}{1 - e^{-r \times b}}\right) \times \mid \hat{\psi}(r)\rangle = E' \times \mid \hat{\psi}(r)\rangle \tag{45}$$

$m_{isoelec}$ and $p_{isoelec}$ are the mass and momentum of isoelectronium respectively, V' reflects the absorption of the repulsive Coulomb potentials by

the much stronger attractive Hulthén potential and since there is only one distance variable we have dropped the subscripts 12 to r.

The equations (44) and (45) exhibit new attractive force holding together strongly the neutral atoms of hydrogen molecule, which is absent in the conventional quantum chemistry. It also permits exact representations of the binding energy and other molecular characteristics. Main features of the above equation are that, it yields much faster convergence of series with much reduced computer times, and resolves other insufficiencies of conventional models.

4.2.2 A three-body isochemical model

In isotopic model, the two electrons are bonded together in a singlet state called isoelectronium. The charge radius of the isoelectronim is sufficiently small and we can assume,

$$r_{12} \leq r_{1A} \text{ and } \quad r_{1B}, \quad r_{12} \approx 0$$
$$r_{1A} \approx r_{2A} = r_A \text{ and } r_{1B} \approx r_{2B} = r_B$$

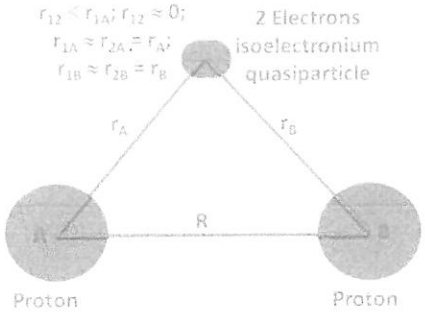


Figure 8: Schematic representation of three-body model of hydrogen molecule.

Moreover, the nuclei are about 2000 times heavier than the isoelectronium. Therefore, equation (45) can be reduced to a restricted three-body

problem similar to that of H_2^+-ion, but not for conventional H_2 molecule. Its final representation with nonunitary transform reads as [4–6],

$$\left(\frac{p_A^2}{2\times m_{prot}}+\frac{p_B^2}{2\times m_{prot}}+\frac{p_{isoelec}^2}{2\times m_{isoelec}} -V'\times\frac{e^{-r\times b}}{1-e^{-r\times b}}\right)\times\mid\hat{\psi}(r)\rangle=E'\times\mid\hat{\psi}(r)\rangle \quad (46)$$

where m_{prot} is the mass of a proton and p_A and p_B are the momenta of protons.

This three-body model of hydrogen molecule consists of two H-protons at rest at a fixed mutual distance plus an isoelectronium moving around them in a oo-shaped orbit Figure 5, according to the structural equation (44) or (46).

An exact variational solution was first studied by Aringazin and Kucherenko [12] and further its exact analytical solution was achieved by Pérez-Enríquez, Marín and Rirera [13].

This model permits for the first time the achievement of an exact solution of H_2 molecule as in the case of H_2^+-ion. It is to be noted that the above exact solution is only possible for the case of the isoelectronium fully stable at short mutual distances. If the mutual distance of the valence electrons no longer restricted to 1 fm, the model is full four- body structure, which as such, does not provide exact solution.

5 Santilli-Shillady Isochemical Model for Water Molecule

Subsequent to the successful study of the isochemical molecular model of isoelectronium for Hydrogen molecule in the historical paper of (1999) [8], Santilli and Shillady proposed their second historical study [14] of hadronic chemistry for the water molecule resulting from the first axiomatic unadulterated principles of binding energy, sign and values of electric and magnetic moments and other data.

Let us consider a water molecule with stable two isoelectronia. For the water molecule we have the following experimental data [6]. The energy

of formation of the water molecule from hydrogen and oxygen atoms is - 9.511 eV, the binding energy is - 10.086 eV, the dissociation energy of the first step production of H + O-H is 5.11 eV and that for the second step production of H + O is 4.40 eV.

Santilli and Shillady in their isochemical model of water molecule (H_2O = H-O-H) assumed that the molecule is at 0^0C in the absence of any rotational, oscillation or other motion. The main hypothesis is that each electron from two H atoms couples in singlet with one 2p electron from the O-atom, resulting in two isoelectronia, one per each bond as shown in Figure 9.

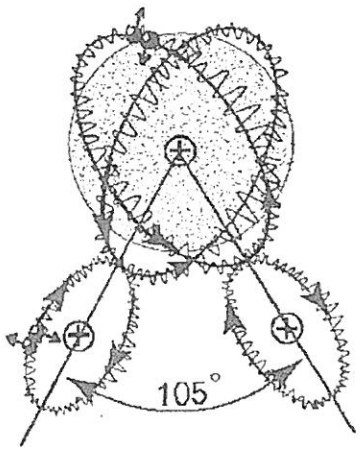


Figure 9: Schematic representation of two isoelectronia of a water molecule.

The conventional Schrödinger equation of H-O molecule or rather bond with the oxygen assumed to have only one elementary charge + e (all other nuclear protons have been assumed as screened by the seven extra-nuclear elecrons) in the nucleus is given by,

$$\left(\frac{1}{2\mu_1}p_1 \times p_1 + \frac{1}{2\mu_2}p_2 \times p_2 + \frac{e^2}{r_{12}} - \frac{e^2}{r_{1A}} - \frac{e^2}{r_{2A}} - \frac{e^2}{r_{1B}} - \frac{e^2}{r_{2B}} + \frac{e^2}{R}\right) \times \mid \psi\rangle = E \times \mid \psi\rangle \qquad (47)$$

where, the sub-indices represent 1 and A the hydrogen, 2 and B the oxygen, prior to the indicated screening and in the absence of all hadronic effects.

Now subjecting the above model to a transform, which is nonunitary only at the short mutual distances $r_c = b^{-1} = r_{12}$ of the two valence electrons (here assumed to be hadronic horizon), and becomes unitary at larger distances, that is we have,

$$\hat{I}_{r\leq 10^{-10}\mathrm{cm}} \neq I, \quad I_{r\gg 10^{-10}\mathrm{cm}} = I \tag{48}$$

It is further assumed that the state and related Hilbert space of systems (equation (47)) can be factorized as (herein each term is duly symmetrized or antisymmetrized),

$$\mid \psi\rangle = \mid \psi_{12}\rangle \times \mid \psi_{1a}\rangle \times \mid \psi_{1b}\rangle \times \mid \psi_{2a}\rangle \times \mid \psi_{2b}\rangle \times \mid \psi_R\rangle, \tag{49}$$

$$\mathcal{H}_{Tot} = \mathcal{H}_{12} \times \mathcal{H}_{1a} \times \mathcal{H}_{1b} \times \mathcal{H}_{2a} \times \mathcal{H}_{2b} \times \mathcal{H}_R. \tag{50}$$

The nonunitary transform acts only on the r_{12} variable characterizing the isoelectronium while leaving all other variables unchanged. The simplest solution is given by,

$$U(r_{12}) \times U^{\dagger}(r_{12}) = \hat{I} = \exp\left[\frac{\psi(r_{12})}{\hat{\psi}(r_{12})} \int d^3 r_{12} \hat{\psi}^{\dagger}{}_{1\downarrow}(r_{12}) \times \hat{\psi}_{2\uparrow}(r_{12})\right], \tag{51}$$

where the ψ's represent conventional wavefunction and $\hat{\psi}$'s represent the isowavefunctions, for which we have the fundamental condition of fast convergence,

$$\mid \widehat{T} \mid = \mid \left(U \times U^{\dagger}\right)^{-1} \mid \ll 1 \tag{52}$$

We can now construct the isochemical model by transforming short-range terms (isochemistry) and adding un-transformed long range ones, thus resulting in radial equation,

$$\left(-\frac{\hbar^2}{2\times\mu_1}\widehat{T}\times\nabla_1\times\widehat{T}\times\nabla_1 - \frac{\hbar^2}{2\times\mu_2}\widehat{T}\times\nabla_2\times\widehat{T}\times\nabla_2 + \frac{e^2}{r_{12}}\times\widehat{T} - \frac{e^2}{r_{1A}} - \frac{e^2}{r_{2A}} - \frac{e^2}{r_{1B}} - \frac{e^2}{r_{2B}} + \frac{e^2}{R}\right)\times \mid \hat{\psi}\rangle = E\times \mid \hat{\psi}\rangle \tag{53}$$

As Hulhtén potential behaves at small distances like the Coulomb ones equation (53) , without absorbing electrostatic terms in Hulthén one, becomes,

$$\left(-\frac{\hbar^2}{2\times\mu_1}\times\nabla_1^2-\frac{\hbar^2}{2\times\mu_2}\times\nabla_2^2-V'\times\frac{e^{-r_{12}\times b}}{1-e^{-r_{12}\times b}}\right.$$
$$\left.-\frac{e^2}{r_{1A}}-\frac{e^2}{r_{2A}}-\frac{e^2}{r_{1B}}-\frac{e^2}{r_{2B}}+\frac{e^2}{R}\right)\times\mid\hat{\psi}\rangle=E\times\mid\hat{\psi}\rangle \quad (54)$$

The above model can be simplified further. In the first approximation under the assumption that herein considered, the H-O molecule (equation (54)) can be reduced to a restricted three body problem like H_2^+-ion, and we get

$$\left(-\frac{\hbar^2}{2\times\mu_1}\times\nabla_1^2-\frac{\hbar^2}{2\times\mu_2}\times\nabla_2^2-V'\times\frac{e^{-r_{12}\times b}}{1-e^{-r_{12}\times b}}\right.$$
$$\left.-\frac{2e^2}{r_A}-\frac{2e^2}{r_B}+\frac{e^2}{R}\right)\times\mid\hat{\psi}\rangle=E\times\mid\hat{\psi}\rangle \quad (55)$$

The corrections due to the screening of various electrons in the oxygen and other corrections are needed in sensing of O-nucleus by isoelectronium as well as by the H-nucleus yields,

$$\left(-\frac{\hbar^2}{2\times\mu_1}\times\nabla_1^2-\frac{\hbar^2}{2\times\mu_2}\times\nabla_2^2-V'\times\frac{e^{-r_{12}\times b}}{1-e^{-r_{12}\times b}}\right.$$
$$\left.-\frac{2e^2}{r_A}-\frac{2e^2\left(1-e^{-\alpha r_B}\right)}{r_B}+\frac{e^2\left(1+e^{-\alpha R}\right)}{R}\right)\times\mid\hat{\psi}\rangle=E\times\mid\hat{\psi}\rangle \quad (56)$$

where α is positive parameter, E is half of the binding energy of the water molecule and the mass of the isoelectronium, the internuclear distance and the size of the isoelectronium can be fitted from the value of binding energy and other data.

Thus the model admits an exact analytic solution, which exists for the case fully stable isoelectronium. In fact for the unstable isoelectronium, the model becomes four body structure, which as such admits no exact solution. It also exhibits attractive strong force among the neutral atoms of H-O molecule, which is absent in quantum chemistry. It permits an

essentially exact representation of the binding energy, electric and magnetic moments. More importantly the model yields much faster convergence of series with much reduced computer times and resolves other insufficiencies of conventional models.

It has been observed that though Santilli-Shilldy isochemical model of the hydrogen molecule admits an exact analytical solution capable of representing molecular binding energy accurate to sixth place of decimal, the inter nuclear distance is 19.6 % higher than the experimental value.

Table 1: Isoelectronium results for selected molecules

Species	H_2	H_2O	HF
SCF-energy (DH) (a.u.)	-1.132806^a	-76.051524	-100.057186
Hartree-Fock[d] (a.u.)			-100.07185^d
Iso-energy (a.u.)	-1.174411^c	-76.398229^c	-100.459500^c
Horizon R_c (Å)	0.00671	0.00038	0.00030
QMC energy[d,e] (a.u.)	-1.17417	-76.430020^e	-100.44296^d
Exact non-rel. (a.u.)	-1.174174^f		-100.4595^d
Corellation (%)	99.9^b	91.6^b	103.8
SCF-dipole (D)	0.0	1.996828	1.946698
Iso-dipole (D)	0.0	1.847437	1.841378
Exp. dipole (D)	0.0	1.85^g	1.82^g
Time[h] (mins)	0:15.49	10:08.31	6:28.48

[a](DH$^+$) Dunning-Huzinaga (10S/6P), [6,2,1,1,1/4,1,1]+H_2P_1=3D1.
[b]LEAO-6G1S + optimized GLO-2S and GLO-2P.
[c]Relative to the basis set used here, not quite HF-limit.
[d]Iso-energy calibrated to give exact energy for HF.
[e]Hartree-Fock and QMC energies from Luchow and Anderson [33].
[f]QMC energies from Hammond *et al.* [30].
[g]First 7 sig. fig. from Kolos and Wolniewicz [31].
[h]Data from Chemical Rubber Handbook, 61st ed., p. E60.
[i]Run times on an O2 Silicon Graphics workstation (200 MFLOPS max.).

The results based on the isochemical model of Santilli-Shillady are depicted in the Table 1.

6 Magnecules

The discovery of isochemical models of H_2 and H_2O, led Santilli and coworkers to set their research goal to search for altogether new mode of bonding resulting in formation of stable clusters. In early 1998, Santilli introduced his new chemical species called magnecules, having new magnecular bond [5, 15].

Magnecules are novel chemical species having at least one magnecular bond. The magnecules in gases, liquids and solids consist of stable clusters composed of conventional molecules, and/or dimmers and/or individual atoms bonded together with opposing magnetic polarizations of the orbits of at least the peripheral atomic electrons when exposed to sufficiently strong external magnetic fields, as well as the polarization of the intrinsic magnetic moments of nuclei and electrons. The atoms are held together by magnetic fields originating due to toroidal polarization of the atomic electron orbits. The rotation of the electrons within the toroid creates the magnetic field which is absent for the same atom with conventional spherical distribution of electrons in orbitals. When two such polarized atoms are sufficiently close to each other and in north-south, north-south alignment, the resulting total force between the two atoms is attractive. The polarization is brought about by high magnetic field which is obtained such as in the case of high voltage DC arc. Magnecules have been synthesized by Santilli and coworkers between identical or non-identical molecules. These magnecules and magneplexes have found applications as clean fuels [5, 6].

6.1 Classification of Magnecules

There are a host of magnecules, magneplexes and magneclusters synthesized by Santilli and co-workers. For example, Santilli proposed that the species H_3 and O_3 have a magnecular structure of the type $H_3 = (H–H)\times H$ and $O_3 = (O–O)\times O$ namely, they comprise ordinary molecules H_2 and O_2 with valence bond (shown by –) plus a third atom with magnecular bond (shown by $\times$). The magnecular bonds have on an average strength of 20-25 kcal/mol [16].

Professor Santilli has proposed the magnecule composed of two hydrogen

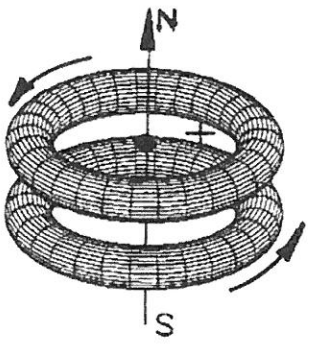


Figure 10: Representation of a magnecule formed by two hydrogen atoms.

atoms as H×H as shown in the Figure 6.2. Whereas, Figure 6.2 given below, shows Professor Santilli's conception of H_3 as H×H×H or H_2×H.

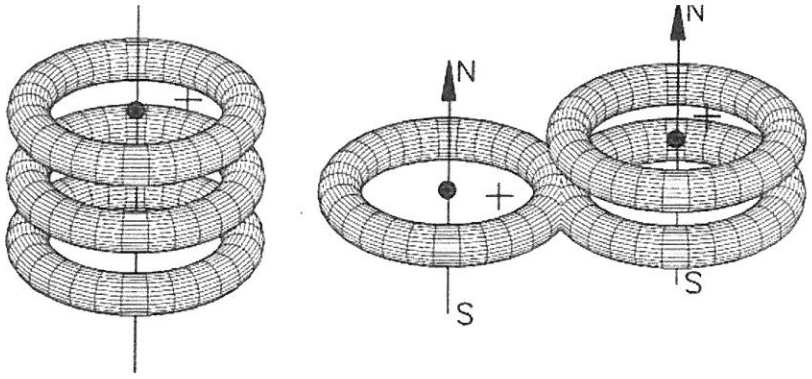


Figure 11: Magnecules having formula H_3. On the left it is formed from 3 H atoms and on the left it is formed with one H atom and one hydrogen molecule.

Magnecules are called elementary when only composed of two molecules; magneplexes when entirely composed of several identical molecules; and magneclusters when composed of several different molecules. The representative examples are given below.

The elementary *magnecules* in liquid state are,

$$\{\text{H–H}\} \times \{\text{H–H}\}, \{\text{O–O}\} \times \{\text{O–O}\} \text{ etc.}$$
$$\{\text{C}_{15} - \text{H}_{20} - \text{O}\} \times \{\text{C}_{15} - \text{H}_{20} - \text{O}\} \text{ etc.}$$

the examples of *magneplexes* in gas and liquid states are,

$$\{\text{H–H}\} \times \{\text{H–H}\} \times \{\text{H–H}\} \times \{\text{H–H}\} \times \cdots\cdots$$
$$\{\text{H–O–H}\} \times \{\text{H–O–H}\} \times \{\text{H–O–H}\} \times \{\text{H–O–H}\} \times \cdots$$

and the examples of *magneclusters* are,

$$\{\text{H–H}\} \times \{\text{C–O}\} \times \{\text{O–C–O}\} \times \{\text{C=O}\} \times \cdots\cdots$$
$$\{\text{C}_{13} - \text{H}_{18} - \text{O}\} \times \{\text{C}_{14} - \text{H}_{12} - \text{O}_3\} \times \{\text{C}_{15} - \text{H}_{20} - \text{O}\} \times \cdots\cdots$$

The generic representation of gas magnecules requires the presence of individual atoms and molecules, as for example,

$$\{\text{H–H}\} \times \{\text{C–O}\} \times \text{H} \times \{\text{H–O–H}\} \times \text{C} \times \{\text{H–O}\} \times \cdots$$

6.2 Experimental Detection and Identification of Magnecules

Professor Santilli has very lucidly described problems and their solution in the unambiguous experimental detection of magnecules [15, 17]. Its brief account is given below. Since magnecules have properties very different from those of conventional molecules, the experimental detection of magnecules requires a special care. In particular, methods which have been conceived and developed for the detection of molecules are not necessarily effective for the detection of the different chemical species of magnecules precisely in view of the basic differences with normal moleculres.

The first indication of a possible gas magnecule is given by MS peaks with large atomic weight which cannot be explained via conventional molecular hypotheses. The second indication of a gas magnecule is given by the lack of identification of said heavy peaks in the MS following a search among all known molecules. A third indication of a gas magnecule then occurs when

said unknown MS peak has no IR signature, except those of its constituents with much smaller atomic weight that occurrence establishes the lack of a valence bond. Final identification of a gas magnecule requires the knowledge of the method used in the production of the gas and other evidence.

As it is the case also for molecules, a serious spectrographic analysis of magnecules requires GC-MS (Gas Chromatography-Mass Spectroscopy) detectors necessarily equipped with IRD (Infrared Detectors), because only such an instrument permits the direct test of the same peaks under both the MS and IR scan. Again, if the IRD operates separately from the GC-MS, the indicated joint inspection is not possible; the IRD can only detect ordinary diatomic bonds; the experimental belief that the MS peak must be a molecule is then consequential. As a concrete example verified later on with actual tests, consider the spectrographic analysis of magnegas. This is a light gas whose heaviest molecule in macroscopic percentages should be the CO_2 at 44 a.m.u. Consider now an MS peak of magnegas at 481 a.m.u. It is evident that, while small deviations could be adapted to quantum chemistry, large deviations of such an order of magnitude cannot be reconciled with established knowledge in a credible way, thus permitting the hypothesis that the MS peak in a light gas with 481 a.m.u. can be a magnecule. The MS scan of the peak soon establishes the impossibility for the computer to identify the peak among all existing molecules. When the GC-MS is equipped with IRD, the analyst can scan the same peak with 481 a.m.u. under the IRD and detect no signature at the 481 a.m.u. value, the only IR signature being that at 44 a.m.u. of the CO_2 as well as those of smaller molecules. The production of the gas under intense magnetic fields then confirm that the peak here considered at 481 a.m.u. is indeed a magnecule composed of a large number of ordinary light molecules, dimers and individual atoms, in accordance with Definition.

Note that the IRD scan in the above test has solely identified conventional molecules without any additional unknown. Yet, the conclusion that the gas considered is solely composed of molecule would be nonscientific for numerous reasons, such as:

1. magnetic bonds are transparent to IR scans with available frequencies;

2. there is no IR detection, specifically, at 481 a.m.u.;

3. IRD do not detect molecules, but only diatomic molecules, chemical groups, radicals, etc.

Therefore, even though the IRD has detected CO_2 in the above test, the actual detection was for the CO bond, in which case the claim of the presence of the full CO_2 molecule is a one opinion, and not the sole one. The anomalous energy content, weight and other features of magnegas confirm the above conclusions, because the latter can only be explained by assuming that a certain percentage of IR counts is indeed due to the carbondioxide molecules, while the remaining percentage is due to unpaired diatomic units of CO trapped in the magnecules. The freeing of these diatomic units and atoms at the time of the combustion, and their recombination into molecules as say as

$$C + O \longrightarrow CO + 225\,\text{kcal/mol}$$

then explains the anomalous energy content.

In addition to the above basic requirements, numerous other precautions in the use of the GC-MS equipped with IRD are necessary for the detection of magnecules, such as:

- the MS equipment should permit measurements of peaks at ordinary temperature, and avoid the high temperatures of the GC-MS column successfully used for molecules;
- the feeding lines should be cryogenically cooled;
- the GC-MS/IRD should be equipped with feeding lines of at least 0.5 mm ID;
- the GC-MS should be set to detect peaks at large atomic weights usually not expected; and
- the ramp time should be the longest allowed by the instrument, e.g., of at least 25 minutes.

It should be stressed that the lack of verification of any one of the above conditions generally implies the impossibility to detect magnecules. For

instance, the use of a feeding line with 0.5 mm ID is un-necessarily large for a conventional light gas, while it is necessary for a gas with magnecular structure such as magnegas. This is due to the unique adhesion of the magnecules against the walls of the feeding line, resulting in occluded lines which prevent the passage of the most important magnecules to be detected, those with large atomic weight. Similarly, it is customary for tests of conventional gases to use GC-MS with columns at high temperature to obtain readings in the shortest possible time, since conventional molecules are perfectly stable under the temperatures here considered. The use of such method would equally prevent the test of the very species to be detected, because they have a characteristic Curie Temperature at which all magnetic features are lost. Magnecules are stable at ordinary temperatures and, consequently, the measurements should be carried out at ordinary temperatures.

Along similar lines, recall that GC-MS with a short ramp time are generally used for rapidity of results. Again, the use of such a practice, which has been proven by extensive evidence to be effective for molecules, prevents clear detection of magnecules. If the ramp time is not of the order of 25 minutes, e.g., it is of the order of one minute, all the peaks of magnecules generally combine into one single large peak. In this case the analyst is generally led to inspect an individual section of said large peak. However, in so doing, the analyst identifies conventional molecules constituting the magnecule, and not the magnecule itself.

When these detectors with short ramp times are equipped with IRD, the latter identify the infrared signatures of individual conventional molecules constituting the said large unique peak, and do not identify the possible IR signature of the single large peak itself. Therefore, a GC-MS with short ramp time is basically unsuited for the detection of magnecules because it cannot separate all existing species into individual peaks.

In conclusion, the experimental evidence of the above occurrences establishes the need in the detection of gas magnecules of avoiding, rather than using, techniques and equipment with a proved efficiency for molecules, thus avoiding the use of GC-MS without IRD, with short ramp time, high column temperatures, microscopic feeding lines, and other techniques. On the contrary, new techniques specifically conceived for the detection of magnecules should be worked out.

The conditions for scientific measurements of liquid magnecules via LCMS/ UVD are more stringent than those for gases, because of the great increase, in general, of the atomic weight of liquid magnecules which are generally much larger than the IR of conventionally used feeding lines. This implies the possible erroneous claim that magnecules do not exist because they are not detected by the LC-MS, while in reality the magnecule to be detected could not enter at all into the instrument.

It should be stressed that the methods for the detection and identification of magnecules are at their infancy and numerous issues remained open at spring 2001. One of the open issues relates to several detections in magnegas of IR signatures apparently belonging to complex molecules, such as light hydrocarbons, while such molecules have not been identified in the MS scans. This occurrence creates the realistic possibility that certain complex magnecules may indeed have an IR signature in view of their size. More specifically, as indicated earlier, magnecules are assumed to be transparent to currently available IRD because their inter-atomic distance is expected to be 104 times smaller than the inter-atomic distance in molecules, thus requiring test frequencies which simply do not exist in currently available IRD.

However, such an argument solely applies for magnecules with small atomic weight, such as the elementary magnecules of Figures and . On the contrary, magnecules with heavy atomic weight may well have an IR signature and, in any case, the issue requires specific study. This possibility is confirmed by the fact that magnegas is created via an under-liquid electric arcs whose plasma can reach up to $10{,}000^0$K. The insistence that light hydrocarbons could survive in these conditions, let alone be created, is not entirely clear. This direct observation is confirmed by the fact that no hydrocarbon has been detected in the combustion of magnegas. In fact, the cars running on magnegas (of the R. M. Santilli Foundation) operate without catalytic converter. Direct analysis of the combustion exhaust show a negative count of hydrocarbons, that is, the exhaust contains less hydrocarbons than the local atmosphere which is used for basic calibration of the instrument.

In summary, it is a case in which light hydrocarbons are seemingly indicated by IR scans to exist in small percentages in magnegas, while no

hydrocarbon has ever been identified in the MS scans, no hydrocarbon is expected to survive at the extreme temperatures of the electric arcs used for their production, and no hydrocarbon has been detected in the combustion exhaust. These occurrences illustrate again that the identification of conventional molecules via the sole use of IR scans or, equivalently, the sole use of MS scans, is, in general, is not a conclusive opinion.

Finally we need to acknowledge that Santilli [15] for the first time presented the theoretical and experimental evidence of the existence of magnecules in gases and liquids as described above. He observed that magnecules can be directly verified under microscopic observation to persist at the solid state. The evidence of magnecules in liquids was also obtained by different laboratories using photographic and different spectroscopic technics [17]. Recently Y. Yang and coworkers [18] measured the molecular weight of magnehydrogen using GC-TCD.

6.3 Energetics of Magnecules

The magnecules release energy in thermochemical reactions. This feature is important from the point of view of new clean fuels such as magnegas. This feature is crucially dependent on the existence within magnecules of individual atoms, such as H, C or O and/or individual unpaired molecules such as H–O and H–C. Upon breakdown of these magnecules due to combustion, these individual atoms and molecules coupled themselves into conventional molecules via known exothermic reactions such as,

$$\begin{aligned} H + H &\longrightarrow H_2 + 105\,\text{kcal/mol} \\ C + O &\longrightarrow CO + 225\,\text{kcal/mol} \\ H\text{–}O + H &\longrightarrow H_2O + 28\,\text{kcal/mol} \end{aligned}$$

Thus it would be interesting to investigate the catalytic utility of magnecules and possibly avoid catalyst poisoning at industrial level.

7 Shallow Potential Energy Minima at the Top of the Energy Barrier of Chemical Reactions vis-à-vis isoelectronium

Let us consider the following representative bimolecular chemical reaction,

$$\mathrm{A} + \mathrm{B} \underset{k_r}{\overset{k_f}{\rightleftharpoons}} \mathrm{C} + \mathrm{D} \tag{57}$$

where A and B are the reactants, C and D are the products and k_f and k_r are the forward and reverse rate constants respectively. It is an observed fact that the rates of reactions get enhanced with increase in temperature of the system. Thus it tells us that there exists a potential energy barrier for the crossing over of A and B to produce C and D. The height of the barrier is called Arrhenius activation energy, E_a, of the chemical reaction. Obviously the value of E_a for forward and reverse reactions would be different if the enthalpy of reaction in not zero. This implies that every collision between reactant doesn't produce products. That is most of the collisions between reactants are non-productive and only a fraction of the said collisions are capable of producing products. This fraction is obviously determined by the Boltzmann fraction. Mathematically, it gets expressed as,

$$Rate \propto Z'_{AB} \exp(-(E_a)_f/RT) \tag{58}$$

where Z'_{AB} collision number per second for collisions of A and B, R is the universal gas constant and T is the temperature of the system. This gets lucidly illustrated by Figure 12. Further, the value of Z'_{AB} depends on the concentration of A and B that is we have

$$Z'_{AB} = Z_{AB} \times C_A \times C_B \tag{59}$$

and the law of mass action [19] gives the expression of the forward rate that reads as,

$$Rate = k_f \times C_A \times C_B \tag{60}$$

Hence, from equations (58) - (60) we have,

$$k_f \propto Z_{AB} \times e^{-(E_a)_f/RT} \tag{61}$$

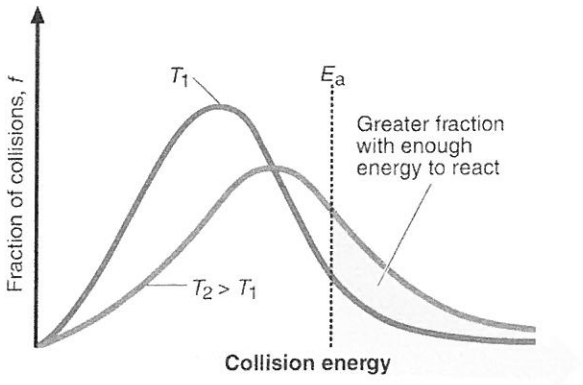


Figure 12: Fraction of bimolecular collisions at two different temperatures with energy of colliding pair.

which has been expressed by Arrhenius as follows,

$$k_f = A_f \times e^{-(E_a)_f/RT} \tag{62}$$

where A_f is the Arrhenius pre-exponential factor of the forward chemical reaction and gets quantified as, $A_f = p_f \times Z_{AB}$ where p_f is the probability factor of the forward chemical reaction. It thus tells us that even if a collision pair possesses the required energy determined by the Boltzmann factor it may not produce the products. This is so because there may be a requirement of an orientation during collision. This in chemical kinetics is termed as steric requirements. It has been shown that the p factor should also account for the statistical requirements and quantum mechanical tunneling wherever they become important. Hence, the value of p can be more than 1 in such cases otherwise it is always less than 1.

Eyring while developing his celebrated *transition state theory of bimolecular reaction rates* considered the configuration of reactants at the top of the barrier as a new chemical species and called it an *activated complex or transition state* [19–22]. In the case that is depicted in Figure 13 the activated complex at the top of the barrier gets represented as $(AB)^{\ddagger}$. It needs to be clarified herein that in many texts instead of reaction coordinate the

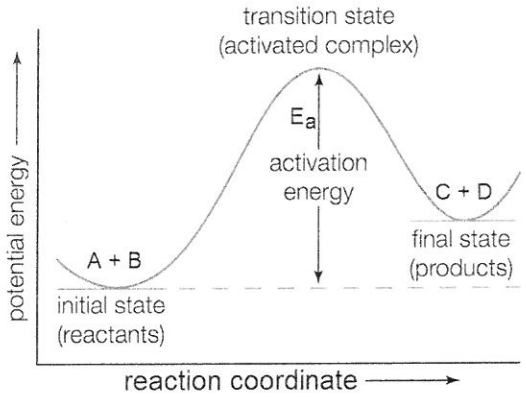


Figure 13: Schematic representation of potential energy curve for an endothermic chemical reaction A + B $\rightleftharpoons$ C + D.

conventional x-axis is labeled as progress of reaction which is totally wrong. This is so because the progress of reaction tells us what percentage of reactants got converted to products. Whereas in Figure 13 one is considering a single colliding pair which till reaching the top of the barrier retain their individual reactant status and at the top of the barrier becomes an activated complex. Also as soon as the activated complex starts climbing down on the other side of the barrier it becomes an union of product molecules and have the individual status of product molecules. In this sense the reaction coordinate is the fourth dimension other than the dimensions determined by x, y, and z axes.

This provided a way to use thermodynamical relations. If we consider that the chemical reaction is being carried out at constant temperature and pressure and using the representation of Figure 13 we are allowed to write,

$$(E_a)_f = H^{\emptyset}_{\ddagger} - (H^{\emptyset}_A + H^{\emptyset}_B)\,, \quad (E_a)_r = H^{\emptyset}_{\ddagger} - (H^{\emptyset}_C + H^{\emptyset}_D) \tag{63}$$

where H are the enthalpies and superscript $\emptyset$ denotes the standard state value. Hence, the standard state enthalpy of the chemical reaction, $\Delta H^{\emptyset}$, is given by,

$$\Delta H^{\emptyset} = (E_a)_f - (E_a)_r = (H^{\emptyset}_C + H^{\emptyset}_D) - (H^{\emptyset}_A + H^{\emptyset}_B) \tag{64}$$

Therefore, from the above discussion it is clear that the molecular configuration of the activated complex at the top of the barrier is determined by the structural and configurational aspects not only of reactants but also of the products it forms. Moreover, in practice the activated complex is a transient state at the top of the barrier. The Arrhenius equation depicting the energy and steric requirements of a chemical reaction in general reads as,

$$k = A \times e^{-E_a/RT} \tag{65}$$

where $A = p \times Z$.

We have given above details to assist reader to appropriately grasp the arguments presented herein.

As there is an energy requirement of a chemical reaction the workers in this field computed potential energy surfaces using quantum mechanics for a large number of elementary chemical reactions. The simplest chemical reaction involving bond breaking and bond forming is $H + H_2 \rightarrow H_2 + H$. For our consideration we are reproducing the potential energy surface for this chemical reaction in Figure 14

Notice that the top of the potential energy barrier corresponds to the saddle point on the potential energy surface of Figure 14. At the same time the saddle point corresponds to a shallow minima of about 3.3 kcal/mol. This is the artifact of the quantum mechanical method adopted for calculating the potential energy at and about the saddle point. Moreover, there have been more sophisticated attempts to recalculate the potential energy of the asserted linear activated complex, those claim higher level of accuracy of the results, but the claim of the said shallow minima at the top of the barrier remained unaffected. For this reaction we need to point out two fundamental aspects one concerns the pre-exponential factor of this reaction and the other is about the physical reality of the shallow minima at the saddle point. Let us discuss the latter aspect first.

But as elaborated above the quantum mechanical calculations of valence bond is not commensurate with the reality and hence Santilli advents the concept of isoelectronium to describe a valence bond in conformity of reality. However, an isoelectronium can be formed only by spin-paired electrons and hence when third atom approaches H_2 molecule at the top of the barrier the resulting union H− − −H− − −H cannot attain even marginal stability

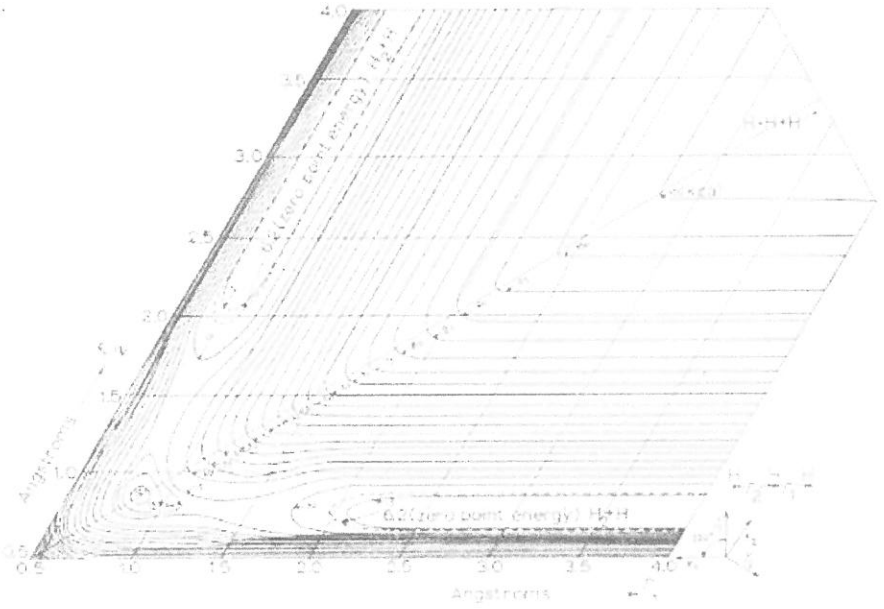


Figure 14: The skewed potential energy contour map surface for co-linear H− − −H− − −H [21].

by lowering its potential energy and this union would be paramagnetic. What can happen at the top of the barrier is simultaneous breaking of old isoelectronium and the formation of a new isoelectronium. In this process energy cannot get first liberated even marginally and thereafter entirely absorbed as the new isoelectronium is formed. In order to happen this a third body is required to extract energy from H− − −H− − −H union and immediately after that yet another third body is required to supply exactly same amount of energy. In case this happens the rate of chemical reaction should depend upon the concentration of say of an inert constituent. However, such dependence of reaction rate has not been observed nor the order of reaction gets changed on addition of inert gas.

However, from magnetostatic interactions point of view which generates strong attractive force between two electrons within 1fm distance. We see

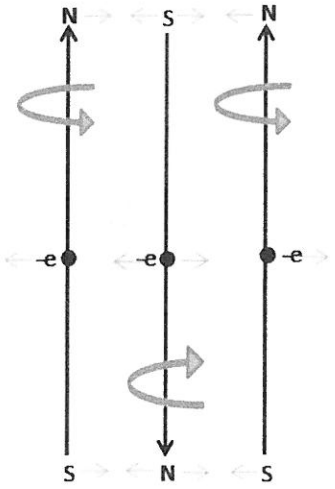


Figure 15: The schematic depiction of the activated complex at the top of the potential energy barrier with its elctrostatic and magnetostatic interactions for the linear H− − −H− − −H configuration.

that as H atom approaches near H_2 molecule at the top of the energy barrier the process that occurs is the start of weakening of existing overlap of wavepackets of isoelectronium of H_2 molecule and simultaneous strengthening of overlap begins of wavepackets of the electrons of the approaching H atom and the central H atom. That is at the top of the barrier the central H-atom simultaneously experiences magnetostatic attraction from both the left and right H-atoms (see Figure 15). That does not offer an opportunity to even marginally stabilize H− − −H− − −H union at the top of the energy barrier. Moreover, the transient existence of H− − −H− − −H cannot be considered as three electron isoelectronium because it would be a triplet union that forbids any stabilization. Hence, we conclude that the claimed shallow minimum at the top of the barrier is a fallacious outcome of quantum chemistry.

From the fact that an isoelectronium is broken and a new isoelectronium is formed in this chemical reaction it implies that only those collisions having the required energy would form the activated complex in which the

spin of the approaching H atom must be opposite to that of the H atom of the H_2 molecule lying on its. This is an additional restriction that would determine the value of pre-exponential factor of this chemical reaction. This is a new aspect that also determines the pre-exponential factor or the probability factor p of this reaction. In fact this factor plays an essential role in determining the p factor of all chemical reactions in which a new covalent bond is formed.

8 Concluding remarks

In this paper we have reviewed the work of Professor Santilli on the hadronic chemistry energetics of hydrogen and water molecules in adequate details [4]. Then we have discussed the energetic aspects of Santilli's magnecules [6]. Finally, we have taken this opportunity to apply the concept of isoelectronium to ascertain the stability of activated complex, identified in Eyring's transition state theory of bimolecular reaction rates [19–22], which is a transient state producing products. Our investigation does not support the shallow minima obtained by conventional quantum mechanics for the activated complex at the top of the barrier.

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DOES AN INITIAL NON PATHEOLOGICAL SINGULARITY AFFECT DIFFERENTIATION BETWEEN EITHER A SINGLE UNIVERSE OR A MULTIVERSE?

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Abstract

First, we assume a classical 4 dimensional repeating universe, so the initial radius $R_{initial} \to 0$ if Stoica actually derived Einstein equations in a formalism which remove the big bang singularity pathology holds . We present in the first case if there is a single universe the following results. Results specifically stating that entanglement entropy in the early universe exists with a shrinking scale factor, due to Muller and Lousto , and show that there are consequences due to initial entanged $S_{Entropy} = .3r_H^2/a^2$ for a time dependent horizon radius r_H in cosmology, with (flat space conditions) $r_H = \eta$ for conformal time . Even if the spatial length goes to zero. Then, we state that the presence of computational bits is necessary for cosmological evolution and also that the presence of computational bits affects determining a difference between a single universe or a multiverse. For reasons presented in this document a multiverse would probably preclude $R_{initial} \to 0$ for reasons alluded to by Kauffman's article whose main result we adopt.

Keywords: Fjortoft theorem, thermodynamic potential, matter creation, vacuum energy
non pathological singularity affecting Einstein equations,planck length, multiverse, Kauffman conjecture

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1. **Introduction** This article starts off with a single universe construction which preserves a minimum non zero 'cosmological' vacuum energy Λ , and in doing so keep the bits, for computational bits cosmological evolution even if in four dimensions we have the initial radius R*initial*→vanishing value. We also find that in the case of a multiverse, that such considerations may not hold and that cosmic singularities have a different characteristic in the multiverse setting than in the single universe repeated over and over again. i.e. using an argument borrowed and modified from Kauffman[13], the multiverse will not mandate 'perfect' singularities. The existence of a multiverse may allow for non zero singularities in lieu with the Kauffman argument[1] cited at the end of the document, plus the lower pre big bang temperatures which may allow for the survivial of gravitons just before the onset of the cosmological expansion phase. Note, that the supposition is that in a multiverse, that one would NOT have R*initial*→vanishing value for reasons stated in the manuscript. We also will be examing a multiverse generalization of the Penrose CCC hypothesis [24]for reasons given

2. Review of what happens with cosmological' vacuum energy Λ in the single repeating universe case. Here, R*initial*→vanishing

This article initially for a SINGLE repeating universe investigates what happens physically if there is a non pathological singularity in terms of Einsteins equations at the start of space-time. This eliminates the necessity of having then put in the Planck length since then ther would be no reason to have a minimum non zero length. The proposal come from [27] by Stoica who may have removed the reason for the development of Planck's length as a minimum safety net to remove what appears to be pathologies at the start of applying the Einstein equations at a space-time singularity, and are commented upon in this article. $\rho \sim H^2 / G \Leftrightarrow H \approx a^{-1}$ in particular is remarked upon. This is different from the Fjoroft case given in Appendix I below.. The idea is that entanglement entropy will help generate bits, due to the presence of a vacuum energy, as derived at the end of the article, and the presence of a non-zero vacuum energy value, is necessary for cosmological evolution. Before we get to that creation of what is a necessary creation of vacuum energy conditions we refer to constructions leading to extremely pathological problems which [27] could lead to minus the presence of initial non zero vacuum energy. Also, reference [3] adds more elaboration on this. Note a change in entropy formula given by Lee [14] about the inter relationship between energy, entropy and temperature as given by

$$m \cdot c^2 = \Delta E = T_U \cdot \Delta S = \frac{\hbar \cdot a}{2\pi \cdot c \cdot k_B} \cdot \Delta S \tag{1}$$

Lee's formula is crucial for what we will bring up in the latter part of this document. Namely those changes in initial energy could effectively vanish if [27] is right, i.e. Stoica removing the non-pathological nature of a big bang singularity. That is, unless entanglement entropy is used.

If the mass m, i.e. for gravitons is set by acceleration (of the net universe) and a change in entropy $\Delta S \sim 10^{38}$ between the electroweak regime and the final entropy value of, if $a \cong \frac{c^2}{\Delta x}$ for acceleration is used, so then we obtain

$$S_{Today} \sim 10^{88} \tag{2}$$

Then we are really forced to look at Eq. (1) as a paring between gravitons (today) and gravitinos (electro weak) in the sense of preservation of information.

Having said this note by extension $\rho \sim H^2/G \Leftrightarrow H \approx a^{-1}$. As ρ changes due to $\rho \sim H^2/G$ and $R_{initial} \sim \frac{1}{\#}\ell_{Ng} < l_{Planck}$, t hen a is also altered i.e. goes to zero.

What will determine the answer to this question is if $\Delta E_{initial}$ goes to zero if $R_{initial} \to 0$ which happens if there is no minimum distance mandated to avoid the pathology of singularity behavior at the heart of the Einstein equations. In doing this, we avoid using the energy $E \to 0^+$ situation, i.e. of vanishing initial space-time energy, and instead refer to a nonzero energy, with $\Delta E_{initial}$ instead vanishing. In particular, the Entanglement entropy concept as presented by Muller and Lousto [17] is presented toward the end of this manuscript as a partial resolution of some of the pathologies brought up in this article before the entanglement entropy section. No matter how small the length gets, $S_{entropy}$ if it is entanglement entropy, will not go to zero. The requirement is that the smallest length of time, t, rescaled, does not go to zero. This preserves a minimum non zero Λ vacuum energy, and in doing so keep non zero amounts of initial bits, for computational bits cosmological evolution even if $R_{initial} \to 0$ Before doing that, we review Ng [7 to 18] and his quantum foam hypothesis to give conceptual underpinnings as to why we later even review the implications of entanglement entropy. I.e. the concept of bits and computations is brought up because of applying energy uncertainty, as given by [18] and the Margolis theorem appears to indicate that the universe could not possibly evolve if [27] is applied, in a 4 dimensional closed universe. This bottle neck as indicated by Ng's [18] formalism is even more striking in the author's end of article proof of the necessity of using entanglement entropy in lieu of the conclusion involving entanglement entropy, which can be non-zero, even if $R_{initial} \to 0$ provided there is a minimum non zero time length.

3. Review of Ng, [18] with comments.

First of all, Ng refers to the Margolus-Levitin theorem with the rate of operations $< E/\hbar \Rightarrow \#operations < E/\hbar \times time = \frac{Mc^2}{\hbar} \cdot \frac{l}{c}$. Ng wishes to avoid black-hole formation $\Rightarrow M \le \frac{lc^2}{G}$. This last step is not important to our view point, but we refer to it to keep fidelity to what Ng brought up in his presentation. Later on, Ng[18] refers to the $\#operations \le (R_H/l_P)^2 \sim 10^{123}$ with R_H the Hubble radius. Next Ng refers to the $\#bits \propto [\#operations]^{3/4}$. Each bit energy is $1/R_H$ with $R_H \sim l_P \cdot 10^{123/2}$

The key point as seen by Ng [18] and the author is in

$$\#bits \sim \left[\frac{E}{\hbar}\cdot\frac{l}{c}\right]^{3/4} \approx \left[\frac{Mc^2}{\hbar}\cdot\frac{l}{c}\right]^{3/4} \tag{3}$$

Assuming that the initial energy E of the universe is not set equal to zero, which the author views as impossible, the above equation says that the number of available bits goes down dramatically if one sets $R_{initial} \sim \frac{1}{\#}\ell_{Ng} < l_{Planck}$? Also Ng writes entropy S as proportional to a particle count via N.

$$S \sim N \cong \left[R_H/l_P\right]^2 \tag{4}$$

We rescale R_H to be

$$R_H\big|_{rescale} \sim \frac{l_{Ng}}{\#} \cdot 10^{123/2} \tag{5}$$

The upshot is that the entropy, in terms of the number of available particles drops dramatically if # becomes larger.

So, as $R_{initial} \sim \frac{1}{\#} \ell_{Ng} < l_{Planck}$ grows smaller, as # becomes larger

a. The initial entropy drops
b. The number of bits initially available also drops.

The limiting case of (4) and (5) in a closed universe, with no higher dimensional embedding is that both would almost vanish, i.e. appear to go to zero if # becomes very much larger. The quest4ion we have to ask is would the number of bits in computational evolution actually vanish?

4. Does it make sense to talk of vacuum energy if $R_{initial} \neq 0$ is changed to $R_{initial} \to 0$? Only answerable straightforwardly if an embedding superstructure is assigned. Otherwise difficult. Unless one is using entanglement entropy which is non zero even if $R_{initial} \to 0$

We summarize what may be the high lights of this inquiry leading to the present paper as follows.

4a. One could have the situation if $R_{initial} \to 0$ of an infinite point mass, if there is an initial nonzero energy in the case of four dimensions and no higher dimensional embedding even if [27] goes through verbatim. The author sees this as unlikely. The infinite point mass construction is verbatim if one assumes a closed universe,. with no embedding superstructure and no entanglement entropy..The author, in lieu of the manuscript sees no reason as to what would perturb this infinite point structure, so as to be able to enter in a big bang era. In such a situation, one would not have vacuum energy unless entanglement entropy was used. That is unless one has a non-zero entanglement entropy [17] present even if $R_{initial} \to 0$. See reference [16] for a presentation of a similar argument.

4b. The most problematic scenario. $R_{initial} \to 0$ and no initial cosmological energy. I.e. in a 4 dimensional closed universe. Then there would be no vacuum energy at all.initially. This example is an initially empty initial state, not held to be plausible by Volovik[28]

4c. If additional dimensions are involved in beginning cosmology, than just 4 dimensions will lead to physics which may give credence to other scenarios. One scenario being the authors speculation as to initial degrees of freedom reaching up to 1000, and the nature of a phase transition from essentially very low degrees of freedom, to over 1000 as speculated by the author in 2010 [2].

4d. What the author would be particularly interested in knowing would be if actual semiclassical reasoning could be used to get to an initial prequantum cosmological state. This would using [12], as well as using [12 to 6] and [13 to 7] , with both these last references relevant to forming Planck's constant from electromagnetic wave equations. The author points to the enormous Electromagnetic fields in the electroweak era as perhaps being part of the background necessary for such a semi classical derivation, plus a Octonionic space-time regime, as before inflation flattens space-time, as forming a boundary condition [4]

The relevant template for examinging such questions is given in the following table 1 .

4e. The meaning of Octonionic geometry prior to the introduction of quantum physics presupposes a form of embedding geometry similar to Penrose's cyclic conformal cosmology.

4f. Note that a semiclassical argument can be used to construct Table 1 below. In particular, we look at how Planck's constant is derived, as in the electroweak regime of space-time, for a total derivative [6,7]

$$E_y = \frac{\partial A_y}{\partial t} = \omega \cdot A_y' \left(\omega \cdot (t - x)\right) \tag{6}$$

Similarly [2,12]

$$B_z = -\frac{\partial A_y}{\partial x} = \omega \cdot A_y' \left(\omega \cdot (t - x)\right) \tag{7}$$

The A field is part of the Maxwell's equations given by [12] as, when $[\ ]$ represents a D'Albertain operator, that in a vacuum, one would have for an A field [6, 7]

$$[\ ]A = 0 \tag{8}$$

And for a scalar field ϕ

$$[\ ]\phi = 0 \tag{9}$$

Following this line of thought we then would have an energy density given by, if ε_0 is the early universe permeability [6]

$$\eta = \frac{\varepsilon_0}{2} \cdot \left(E_y^2 + B_z^2\right) = \omega^2 \cdot \varepsilon_0 \cdot A_y'^2 \left(\omega \cdot (t - x)\right) \tag{10}$$

We integrate (10) over a specified E and M boundary, so that, then we can write the following condition namely [2,12].

$$\int\int\int \eta\, d(t - x)\, dy\, dz = \omega \varepsilon_o \int\int\int A_y'^2 \left(\omega \cdot (t - x)\right) d(t - x)\, dy\, dz \tag{11}$$

(11) would be integrated over the boundary regime from the transition from the Octonionic regime of space time, to the non Octonionic regime, assuming an abrupt transition occurs, and we can write, the volume integral as representing [6,7]

$$E_{gravitational-energy} = \hbar \cdot \omega \tag{12}$$

Then by applying [6, 7] we get $\hbar$ formed by semi classical reasons in semi classical reasoning similar to [28]

$$\hbar(t) \xrightarrow[Apply\text{-}Machs\text{-}Relations]{} \hbar_P (\text{Constant value}) \tag{13}$$

Then the question we can ask, is that can we have a prequantum regime commencing for .(11) and (12) for $\hbar$ if $R_{initial} \sim \frac{1}{\#}\ell_{Ng} < l_{Planck}$? Is a closed 4 dimensional universe feasible and possible ? If so, then what is the necessary geometrical regime of space-time so that the integration performed in (11) can commence properly? Also, what can we say about the formation of (12) above, as a number, # gets larger and larger, effectively leading to. Also, with an Octonionic geometry regime which is a pre quantum state.[4]

TABLE 1

.Time Interval	Dynamical consequences	Does QM/WdW apply?
Just before Electroweak era	Form $\hbar$ from early E & M fields, and use Maxwell's Equations with necessary to implement boundary conditions created from change from Octonionic geometry to flat space	NO
Electro-Weak Era	$\hbar$ kept constant due to Machian relations	YES
Post Electro-Weak Era to today	$\hbar$ kept constant due to Machian relations	YES Wave function of Universe

Note that the formation period for $\hbar$ is our pre-quantum regime. This table 1 could even hold if $R_{initial} \to 0$ but that the 4 dimensional space-time exhibiting such behavior is embedded in a higher dimensional template. That due to $R_{initial} \to 0$ not removing entanglement entropy as is discussed near the end of this article.

5. If $R_{initial} \to 0$ **then if there is an isolated, closed universe, there is a disaster unless one uses entanglement entropy.**

Otherwise in this case, 5 , one does not have initial entropy, and the number of bits initially disappears.

Abandoning the idea of a completely empty universe, this unperturbed point of matter-energy appears to be a static point with no perturbation, as may be the end result of Fjortoft theorem [25] applied to the thermodynamic potential in [19], i.e. the non definitive anwer for fufillment of criteria of instability by applying Fjortoft's theorem [25] to the potential [19] leading to no instability as given by the potential given in [19] may lead to a point of space-time with no change, i.e. a singular point with 'infinite' mass which does not change at all. This issue will be reviewed in [9] a different procedure, i.e. a so called nonsingular universe construction. To get there we will first impliment [9].

6. Muller and Lousto Early universe entanglement entropy, and its implications. Solving the spatial length issue, provided a minimum time step is preserved in the cosmos,.

We look at [17]

$S_{Entropy} = .3r_H^2/a^2$ for a time dependent horizon radius r_H in cosmology (14)

(14) above was shown by the author to be fully equivalent to

$$S_{Entropy} = .3r_H^2/a^2 \sim \frac{.3}{a^2}\exp\left[-t\cdot\sqrt{\frac{\Lambda}{3}}\right] \tag{15}$$

i.e.

$$\left[-t\sqrt{\frac{\Lambda}{3}}\right] \sim \ln_e\left(\frac{a^2}{.3}\cdot S_{entropy}\right) \tag{16}$$

So, then one has

$$\Lambda \approx \frac{3}{t^2}\cdot\left[\ln_e\left(\frac{a^2}{.3}\cdot S_{entropy}\right)\right]^2 \tag{17}$$

No matter how small the length gets, $S_{entropy}$ if it is entanglement entropy, will not go to zero. The requirement is that the smallest length of time, t, re scaled does not go to zero. This preserves a minimum non zero Λ vacuum energy, and in doing so keep the non-zero initial bits, for computational bits contributions to evolving space time behavior *even if* $R_{initial} \to 0$

7. Reviewing a suggestion as to how to quantify the shrinkage of the scale factor and its connections with entanglement entropy.

We are given by [9] if there is a nonsingular universe, a template as to how to evaluate scale factor a against time scaled over Planck time, with the following results.

$$\ln_e a + \frac{a^6}{6} + \frac{2\cdot a^3}{3} = \sqrt{\frac{8\pi}{3}}\cdot\frac{t}{t_{Planck}} \tag{18}$$

Two time and scale factor values in tandem particularly stand out. Namely,

$$a \sim \frac{a_{scale}}{\left[a_{Planck} \sim 10^{-25}\right]} \equiv 1.344 \Leftrightarrow t \propto t_{Planck} \sim 5.4\times10^{-44}\ \text{sec} \tag{19}$$

Also

$$a \sim \frac{a_{scale}}{\left[a_{Planck} \sim 10^{-25}\right]} \equiv .7414 \Leftrightarrow t \propto 0^+ \tag{20}$$

The main thing we can take from this, is to look at the inter-relationship of how to pin down an actual initial Hubble "constant" expansion parameter, where we look at:

$$1.813 = \exp(H_{Planck} \cdot t_{Planck}) \Leftrightarrow H_{Planck} = \frac{\ln_e(1.813)}{t_{Planck}} \tag{21}$$

Recall that $\Lambda \approx \frac{3}{t^2} \cdot \left[\ln_e \left(\frac{a^2}{.3} \cdot S_{entropy} \right) \right]^2$, which is predicated upon , if the time is close to Planck time the initial maximal density of

$$\rho_{Planck} \sim 5.2 \times 10^{96} kg / m^3 \tag{22}$$

And length given by

$$Length(Planck) = l_{Planck} \sim 1.6 \times 10^{-35} meters \tag{23}$$

So (22) is implying that the amount of matter in a region of space $(l_{Planck})^3$ is initially

$$\rho_{initial} \sim 2 \times 10^{-10} Kg \sim 2 \times 10^{-7} grams \tag{24}$$

Using 1 GeV/c^2 = 1.783×10^{-27} kg means that (24) above is

$$\rho_{initial} \sim 2 \times 10^{-10} Kg \sim 2 \times 10^{-7} grams \sim 10^{+17} GeV \tag{25}$$

Then if

$$10^{+17} GeV \sim \Lambda \approx \frac{3}{t^2} \cdot \left[\ln_e \left(\frac{a^2}{.3} \cdot S_{entropy} \right) \right]^2 \tag{26}$$

It will lead to

$$10^{+17} GeV \times 10^{-70} \sec^2 \sim \left[\ln_e \left(\frac{a^2}{.3} \cdot S_{entropy} \right) \right] \tag{27}$$

Then, to first order, one is looking at Initial entropy to get a non-zero but definite vacuum energy as leading to entanglement entropy of about (just before the electro weak regime)

$$S_{entropy} \sim 1/a^2 \sim 10^{20} - 10^{40} \tag{28}$$

8. 1st level Conclusion if one has a single repeating universe. Making computational bits, via Eq. (18).

As stated by Ng [18] the idea would be to have to give inputs into (3)
Here in this case, even if the spatial contribution, due to [13] goes to zero, the idea would be to have the time length non zero so as to have a space-time version of l non-zero. . This would also be in tandem with calling energy E, in (3) proportional to $\Lambda \approx \frac{3}{t^2} \cdot \left[\ln_e \left(\frac{a^2}{.3} \cdot S_{entropy} \right) \right]^2$, where if the time is Planck time,

in minimum value, and $S_{entropy} \sim 1/a^2 \sim 10^{20} - 10^{40}$ in value, one would have before the electro-weak an input into E, which would require entropy (entanglement)

What remains to be seen is, if there is a geometric sheet in more than 4 dimensions, allowing for non-zero time, as argued for $\Lambda \approx \frac{3}{t^2} \cdot \left[\ln_e \left(\frac{a^2}{.3} \cdot S_{entropy} \right) \right]^2$, even if the spatial component goes to zero, according to [27]. We suggest an update as to what was written by Seth Lloyd [15] with

$$I = S_{total} / k_B \ln 2 = \left[\#operations \right]^{3/4} = \left[\rho \cdot c^5 \cdot t^4 / \hbar \right]^{1/4} \tag{29}$$

when [23]

$$\rho \equiv T^{00} \sim \Lambda_{vacuum-energy} \tag{30}$$

While doing this, a good thing to do, would be to keep in mind the four dimensional version of vacuum energy as given by Park, [22] namely

$$\Lambda_{4-\dim} \approx c_2 \cdot T^{\beta} \tag{31}$$

As well as the transition given by a combination of [22], with [1], Barvinskey et. al.

$$\Lambda_{4-\dim} \propto c_2 \cdot T \xrightarrow[graviton-production]{} 360 \cdot m_P^2 << c_2 \cdot \left[T \approx 10^{32} K \right. \tag{32}$$

Quantifying the above, and giving it experimental proof, via detector technology may allow us to investigate an old suggestion by the author as to four dimension and five dimensional vacuum energy which was given for small time values $t \approx \delta^1 \cdot t_P, 0 < \delta^1 \leq 1$ and for temperatures sharply lower than $T \approx 10^{12} Kelvin$, Beckwith [5] , where for a positive integer n as was written in [5] by the author as given by Eq.(33) below.

$$\frac{\Lambda_{4-\dim}}{\left| \Lambda_{5-\dim} \right|} - 1 \approx \frac{1}{n} \tag{33}$$

In particular, the author is interested in investigating if the following is true, i.e.

Look at an argument provided by Padmanabhan [20], leading to the observed cosmological constant value suggested by Park [22]. Assume that $l_P \sim 10^{-33} cm \xrightarrow[Quantum-Gravity-threshold]{} \tilde{N}^{\alpha} \cdot l_P$, but that when we make this substitution that $1 \leq \tilde{N}^{\alpha} \leq 10^2$ [21]

$$\begin{aligned} \rho_{VAC} &\sim \frac{\Lambda_{observed}}{8\pi G} \sim \sqrt{\rho_{UV} \cdot \rho_{IR}} \\ &\sim \sqrt{l_{Planck}^{-4} \cdot l_H^{-4}} \sim l_{Planck}^{-2} \cdot H_{observed}^2 \end{aligned} \tag{34}$$

i.e. looking at if

$$\Delta\rho \approx \text{a dark energy density } \sim H^2_{observed}/G \tag{35}$$

Now to make it more interesting:

We can replace $\Lambda_{observed}, H^2_{observed}$ by $\Lambda_{initial}, H^2_{initial}$. In addition we may look at inputs from the initial value of the Hubble parameter to get the necessary e folding needed for inflation, according to

$$E-foldings = H_{initial}\cdot\left(t_{End\,of\,\inf} - t_{beginning\ \ of\,\inf}\right) \equiv N \geq 100 \tag{36}$$
$$\Rightarrow H_{initial} \geq 10^{39} - 10^{43}$$

Leading to

$$a(End-of-\inf)/a(Beginning-of-\inf) \equiv \exp(N) \tag{37}$$

If we set $\Lambda_{initial} \sim c_1 \cdot \left[T \sim 10^{32} Kelvin\right]$ which is a variant of [22] implying a very large initial cosmological constant value, we get in line with what Park [22] suggested for times much less than the Planck interval of time at the instant of nucleation of a vacuum state

$$\Lambda_{initial} \sim \left[10^{156}\right] 8\pi G \approx huge\ \ number \tag{38}$$

9. Case if there is a multiverse. I.e. modification of the Penrose CCC hypothesis.

. Using the formalism given in Peacock [23], page 80, we can make the following scaling argument which will prove useful as to the divergence of the multiverse case, and how there is no longer a convenient singularity to refer to, via Stoica [17] or anyone else Peacock, has it that one can write as follows, namely for a scale factor, with infinitesimally small and representing the initial scale factor in pre Planckian space time (40) Here, the main evolving factor to consider is, Peacock [23] , page 80 with from Eq. (31) above. If so then we have to look at one datum which will be important. Using the formalism given in Peacock [23], page 80 we can make the following scaling argument which will prove useful as to the divergence of the multiverse case, and how there is no longer a convenient singularity to refer to, via Stoica [17] or anyone else

Peacock [23], has it that one can write as follows, namely for a scale factor, with a_0 infinitesimally small and representing the initial scale factor in pre Planckian space time

$$a(t) = a_0 \exp\left[\tilde{\tilde{H}}\cdot t\right] \tag{39}$$

Here, the main evolving factor to consider is, Peacock [23], page 80 with $\Lambda_{\cos-const}$ from Eq. (31) above. If so then we have to look at one datum which will be important. Mainly, how the temperature changes.

$$\tilde{H} = \sqrt{\frac{\Lambda_{cos-const} \cdot c^2}{3}} \tag{40}$$

If the term beta in the coefficient of temperature, T , is zero, we have merely the Einstein vanilla Cosmological constant . If the term beta in the coefficient of temperature, T, is not zero, then we should take a good look at what is done in Weinberg [29] where there is a concerted effort to mix in background viscosity =. But first take note of the Grischuck [11] expression as to GW frequency in the high end, with Temperature approaching Planck values, with behavior due to space-time temperature dependence as given by:" M = mass of 'universe' initially, and R = radius of initial dimensions, with Planck temperature values giving for a single universe, and four dimensions

$$\begin{aligned} f_{Peak} &\approx \left(10^{-3}\,\mathrm{Hz}\right)\cdot\left[\frac{T}{T\mathrm{eV}}\right] \sim 10^{10}\,\mathrm{Hz} \\ &\approx \sqrt{\frac{M}{M_{solar-mass}}}\cdot\sqrt{\frac{90\ \mathrm{km}}{R}} \end{aligned} \tag{41}$$

Then in doing this, we will also consider the case where the temperature is low, which we claim is due to a multiverse, and this will be leading to, for ultra-low initial temperatures, for the "pre big bang, namely if there is a multiverse having[11]

$$f_{Peak} \approx \left(10^{-3}\,\mathrm{Hz}\right)\cdot\left[\frac{T}{T\mathrm{eV}}\right] \sim 10^{-18} - 10^{-10}\,\mathrm{Hz} \tag{42}$$

Furthermore, we can write from Page 163 of Penrose [24] , that, if N ~ S (entropy) as given by Ng [18] for a regular single repeating universe structure, that we will have, for a cyclical universe the following power law relationship. Note that in (44) the abbreviation of F.T. stands for field theory [19,24].

$$\begin{aligned} &\Lambda|_{Today}\,[vacuum-energy] \\ &\sim \frac{c^3}{N^6 G\hbar} \equiv N^{-6}\big|_{value-Today} \approx 10^{-120}\ \text{times } \{\text{FT calculated version of Vacuum energy}\} \\ &\sim 1/S^6_{initially} \end{aligned} \tag{43}$$

I.e. that the cosmological constant is set by the initial release of, maybe, gravitons. i.e. and also note that if one does this that one is able to state that initially low entropy will lead to a tendency, later to a scaled cosmological constant which is today's value.

The question in reaching (44) is, if entropy is commensurate with graviton production as brought up by both Giovanni [10] that then one is looking at thermally induced GW production which may indeed impact the cosmological constant. The question to ask is the following reasonable? I.e. if the frequency range of GW ranges from 10 ^ -19 Hertz to 10 ^ 11 Hertz, then in an expression given by Giovannini , graviton production equals the entire production of the entropy of the present day universe, i.e. by [10] There is an expression where one can have all of entropy generated by a graviton count from

$$\begin{aligned} &S_{Graviton-Today's\,era} \propto V\int_{10^{-19}\,Hertz}^{10^{11}\,Hertz} r(\nu)\cdot\nu^2 d\nu \\ &\cong \left(10^{30}\right)^3\cdot\left(\frac{H_1}{M_{Planck-mass}}\right) \propto 10^{90} \\ &\sim (dif\,f\,erence\ \ of 10^{11}\ \ \ to 10^{-19}\ \ Hertz)^3 \end{aligned} \tag{44}$$

If (44) is defensible as to entropy growth, and gravitons play a role, then the initial temperature may be affected by modeling Gravitons as a particle in a viscous fluid, see Weinberg [29] page 592 with Planck time as of the order of magnitude of a mean free time of collisions of Gravitons in a formation plasma as an imperfect fluid

$$T^{\beta} \sim \left[\frac{15}{4}\cdot\frac{1}{a}\cdot\frac{\eta}{t_{Plank}}\right]^{\beta/4} \propto \left[\frac{15}{4}\cdot\frac{1}{a}\cdot\frac{\eta}{\tau_{graviton}}\right]^{\beta/4} \tag{45}$$

Using this (45), if the viscosity drops, the temperature drops as well. We posit that this will then have immediate consequences for the problem of a multiverse versus a single universe

10. Penrose Cosmology supposition and its tie in to temperature and viscosity as used in Eq. (46)

From Penrose, [24] page 130, we have

$$\begin{aligned} &E = 8\pi\cdot T + \Lambda\cdot g \\ &E = source\ \ for\ \ gravitational\ \ field \\ &T = mass\ \ energy\ \ density \\ &g = gravitational\ \ metric \\ &\Lambda = vacuum\ \ energy, rescaled\ \ as\ \ follows \end{aligned} \tag{46}$$

$$g \xrightarrow[ccc]{} \hat{g} = \hat{\Omega}^2 g \tag{47}$$

The single universe CCC has, then, when black holes (up to a million of them) take in space time from an expanding universe, a 'reverse' conformal re set which Penrose [24] sets as

$$\Omega \xrightarrow[CCC]{} \hat{\Omega} \tag{48}$$

This re set, would tend toward a huge viscosity, as for (45) with a very large initial temperature. The question is, what would happen to this equation, and temperature if there is a multiverse. I.e. the viscosity would drop, and that would lead to low initial pre big bang temperatures, i.e. see the following [24]

$$\Pi = \frac{d\Omega}{\Omega^2 - 1} \xrightarrow[\Omega \to \hat{\Omega}]{ccc} SAME\ \ \frac{d\Omega}{\Omega^2 - 1} \tag{49}$$

This will be generalized in the case of a multi verse as follow. (47) is not really altered, but(49) will have a multi verse interpretation, i.e. for the four dimensional 'domain' universes we will call $\Omega_{\tilde{j}}$

$$\Omega_{input-new-cycle} \simeq \frac{1}{n[number-of-'universes']}\cdot \sum_{\tilde{j}=1}^{n[number-of-'universes']} \Omega_{\tilde{j}} \tag{50}$$

Then, there will be a new mapping, of

$$\Omega_{\tilde{j}}['our-universe'] \longrightarrow \left(\Omega_{input-new-cycle}\right)^{-1} \tag{51}$$

This would, then go to a modification of the Penrose mapping in (50) to read as

$$\frac{d\Omega_{\tilde{j}}}{\Omega_{\tilde{j}}^{\,2}-1} \quad \Omega_{\tilde{j}}[\text{'our-universe'}] \longrightarrow \left(+\,\Omega_{\text{next-new-cycle}}\right)^{-1} \; SAME \; \frac{d\Omega_{\tilde{j}}}{\Omega_{\tilde{j}}^{\,2}-1} \tag{52}$$

Eq.(53) with Eq.(52) are in reality a motivation of Ergodic mixing , i.e. a way to have continual re sets of the initial data, for the purpose of having the same initial conditions again and again, i.e. this is a way of a re set of Planck's constant, and of the fine structure constant without the annoyance of the anthropic principle.

The governing principle behind it would be the Ergodic theorem, i.e. see Dye [8], as an averaging process again and again. In doing so, (51) and (52) would through mixing lead to the same re set again and again, but with one major different consequence than in the single repeating universe case, i.e. there would be a low temperature pre big bang, using (42), instead of (41). This would be a way of having a very different answer as to the character of early universe GW generation, with the multiverse having very low GW frequency, even before red shifting of GW, instead of the high frequency GW predicted by Eq. (41). Next then, we will examine the consequences of the initial starting point of the multiverse recycled starting point. Note the multiverse would likely entail an initially low viscosity, which says low temperature.

11. Reexamining the question of a 'near singularity' in a multiverse

We follow the recent work of Kauffmann [13], which sets an upper bound to concentrations of energy, in terms of how he formulated the following equation put in below as (53). (53) specifies an inter-relationship between an initial radius R for an expanding universe, and a "gravitationally based energy" expression we will call $T_G(r)$which lead to a lower bound to the radius of the universe at the start of the Universe's initial expansion, with manipulations. The term $T_G(r)$is defined via (54) afterwards. We start off with Kauffmann's expression [13]

$$R \cdot \left(\frac{c^4}{G}\right) \geq \int_{|r''|\leq R} T_G(r+r'')d^3r'' \tag{53}$$

Kauffmann [13] calls $\left(\frac{c^4}{G}\right)$ a "Planck force" which is relevant due to the fact we will employ (53) at the initial instant of the universe, in the Planckian regime of space-time. Also, we make full use of setting for small r, the following:

$$T_G(r+r'') \approx T_{G=0}(r) \cdot const \sim V(r) \sim m_{Graviton} \cdot n_{Initial-entropy} \cdot c^2 \tag{54}$$

I.e. what we are doing is to make the expression in the integrand proportional to information leaked by a past universe into our present universe, with Ng [18] style quantum infinite statistics use of

$$n_{Initial-entropy} \sim S_{Graviton-count-entropy} \tag{55}$$

Then (55) will lead to

$$R\cdot\left(\frac{c^4}{G}\right)\geq\int_{|r''|\leq R}T_G\left(r+r''\right)d^3r''\approx const\cdot m_{Graviton}\cdot\left[n_{Initial-entropy}\sim S_{Graviton-\ count-\ entropy}\right]$$

$$\Rightarrow R\cdot\left(\frac{c^4}{G}\right)\geq const\cdot m_{Graviton}\cdot\left[n_{Initial-entropy}\sim S_{Graviton-\ count-\ entropy}\right] \quad (56)$$

$$\Rightarrow R\geq\left(\frac{c^4}{G}\right)^{-1}\cdot\left[const\cdot m_{Graviton}\cdot\left[n_{Initial-entropy}\sim S_{Graviton-count-entropy}\right]\right]$$

Here, $\left[n_{Initial-entropy}\sim S_{Graviton-\ count-\ entropy}\right]\sim 10^5$, $m_{Graviton}\sim 10^{-62}\,grams$, and we set Plank length as:

Planck length = l_{Planck} = **1.616199 × 10^{-35} meters**

where we set $l_{Planck}=\sqrt{\frac{\hbar G}{c^3}}$ with $R\sim l_{Planck}\cdot 10^{\alpha}$, and $\alpha>0$. Typically $R\sim l_{Planck}\cdot 10^{\alpha}$ is about $10^3\cdot l_{Planck}$ at the outset, when the universe is the most compact. The value of *const* is chosen based on common assumptions about contributions from all sources of early universe entropy, and will be more rigorously defined in a later paperWe argue that the above methodology, giving a non zero initial starting point is made especially tendable if one is using a low temperature start, allowing for the existence of prior recycling universes gravitons to play a role, i.e. that in the single universe repeated again and again, there would be real issues as to the survival of the graviton allowing for the conclusion as to (56).

12. Fork in the road. Nonzero radii of start of inflation may be linkable to low temperature pre universe due to multiverse. How to confirm it ?

The author's supposition and argument as to the results of (56) which would be key to identifying if a zero point starting point to inflation were mandatory is akin to the question of could gravity and gravitons exist prior to inflation. If there is a multiverse, , then the answer is likely yes. Hence, (56) would indicate that a 'perfect' singularity is not mandatory. The problem though is that then likely initial relic GW would then be enormously long, ie as given in (42) above. This independent of red shifting.

If one has ultra high gravity waves as created at the big bang, then it is likely that a singularity is mandatory. We also then have referred to Stoica's work as to how this could be squeezed down below the Planck length limit, but itself would not be pathological for the reasons stated above.I.e. confirmation of the two alternatives likely hinges upon determination if ultra high GW are indeed part of the pre inflation to inflationary universe's signal heritage[26]

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Appendix I. Fjortoft theorem:

A **necessary condition for instability** is that if z_* is a point in spacetime for which $\frac{d^2U}{dz^2} = 0$ for any given potential U , then there must be some value z_0 in the range $z_1 < z_0 < z_2$ such that

$$\left.\frac{d^2U}{dz^2}\right|_{z_0} \cdot \left[U(z_0) - U(z_*)\right] < 0 \qquad (1)$$

For the proof, see [25] and also consider that the main discussion is to find instability in a physical system which will be described by a given potential U . Next, we will construct in the boundary of the EW era, a way to come up with an optimal description for U

Appendix II. Constructing an appropriate potential for using Fjortoft theorem in cosmology for the early universe cannot be done. We show why

To do this, we will look at Padamanabhan [19] and his construction of (in Dice 2010) of thermodynamic potentials he used to have another construction of the Einstein GR equations. To start, Padamanabhan [19] wrote

If P_{cd}^{ab} is a so called Lovelock entropy tensor, and T_{ab} a stress energy tensor

$$\begin{aligned} &U(\eta^a) = -4 \cdot P_{ab}^{cd} \nabla_c \eta^a \nabla_d \eta^b + T_{ab} \eta^a \eta^b + \lambda(x) g_{ab} \eta^a \eta^b \\ &= U_{gravity}(\eta^a) + U_{matter}(\eta^a) + \lambda(x) g_{ab} \eta^a \eta^b \\ &\Leftrightarrow U_{matter}(\eta^a) = T_{ab} \eta^a \eta^b ; U_{gravity}(\eta^a) = -4 \cdot P_{ab}^{cd} \nabla_c \eta^a \nabla_d \eta^b \end{aligned} \tag{1}$$

We now will look at

$$\begin{aligned} &U_{matter}(\eta^a) = T_{ab} \eta^a \eta^b \quad ; \\ &U_{gravity}(\eta^a) = -4 \cdot P_{ab}^{cd} \nabla_c \eta^a \nabla_d \eta^b \end{aligned} \tag{2}$$

So happens that in terms of looking at the partial derivative of the top (1) equation, we are looking at

$$\frac{\partial^2 U}{\partial (\eta^a)^2} = T_{aa} + \lambda(x) g_{aa} \tag{3}$$

Thus, we then will be looking at if there is a specified η_*^a for which the following holds.

$$\left[\frac{\partial^2 U}{\partial (\eta^a)^2} = T_{aa} + \lambda(x) g_{aa} \right]_{\eta_0^a}^{*} < 0 \tag{4}$$

$$\left[\begin{aligned} &-4 \cdot P_{ab}^{cd} \left(\nabla_c \eta_0^a \nabla_d \eta_0^b - \nabla_c \eta_*^a \nabla_d \eta_*^b \right) + \\ &T_{ab} \cdot \left[\eta_0^a \eta_0^b - \eta_*^a \eta_*^b \right] + \lambda(x) g_{ab} \cdot \left[\eta_0^a \eta_0^b - \eta_*^a \eta_*^b \right] \end{aligned} \right]$$

What this is saying is that there is no unique point, using this η_*^a for which (4) holds. Therefore, we say there is no official point of instability **of** η_*^a due to (3). The Lagrangian structure of what can be built up by the potentials given in (3) with respect to η_*^a mean that we cannot expect an inflection point with respect to a 2nd derivative of a potential system. Such an inflection point designating a speed up of acceleration due to DE exists a billion years ago [5]. Also note that the reason for the failure for Eq.(4) to be congruent to Fjoroft's theorem is due to

$$\left[\frac{\partial^2 U}{\partial (\eta^a)^2} = T_{aa} + \lambda(x) g_{aa} \right] \neq 0, \; for \; \forall \eta_*^a \; choices \tag{5}$$

ON THE INTERPRETATION OF THE LORENTZ TIME TRANSFORMATION

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Abstract

Einstein gave two conflicting interpretations of the Lorentz transformation for time, $\tau=t\sqrt{(1-v^2/c^2)}$, applied to a moving clock. The first was as a coordinate transformation, which was the basis of its derivation. The second was as a physical slowing effect on the moving clock caused solely by its motion relative to a stationary reference clock. These interpretations are not independent. That is, the Lorentz coordinate transformation cannot be applied during the clock's time of motion without correcting for the lack of synchronization between the moving and stationary clocks resulting from the slowing of the moving clock. Otherwise, the Lorentz transformation gives an incorrect result. In addition, the interpretation as a physical effect has seemingly insurmountable logical difficulties, as it subjects the moving clock to a physical slowing dependent upon an arbitrary inertial reference frame, and which is therefore indeterminable. This interpretation is supported by questionable experimental evidence.

Keywords: Lorentz transformations; Time transformations; Relativity; Special Relativity; Coordinate transformations; Time dilation; Twin paradox.

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After deriving the Lorentz transformations as coordinate transformations, Einstein [1], in section 4, "Physical Meaning of the Equations Obtained in Respect to Moving Rigid Bodies and Moving Clocks", makes the rather astonishing claim that the Lorentz time coordinate transformation,

$$\tau = t\sqrt{(1-v^2/c^2)} = t - (1-\sqrt{(1-v^2/c^2)})t\,, \qquad (1)$$

represents a physical slowing effect on a moving clock due merely to its motion relative to a stationary reference clock.

This interpretation not only has no apparent basis in his derivation, but also contradicts it. Now the clocks are no longer physically synchronized at $t > 0$, so the Lorentz transformation (1) is no longer valid during the time of motion. By Einstein's argument, the time interval of the moving clock measured in its own coordinate system at $t > 0$ is no longer τ, but is decreased by the amount

$$(1-\sqrt{(1-v^2/c^2)})t.$$

That is, the clocks are synchronized at $t = \tau = 0$, but are out of synchronization at $t > 0$ by this amount, so that the time coordinate measured by the moving clock at $t > 0$ in its own coordinate system is not τ, but rather

$$\tau' = \tau - (1-\sqrt{(1-v^2/c^2)})t. \qquad (2)$$

The correct transformation at $t > 0$ then becomes

$$\tau' = (t- (1- \sqrt{(1-v^2/c^2)}t) - (1- \sqrt{(1-v^2/c^2)})t, \text{ or}$$

$$\tau' = t - 2(1- \sqrt{(1-v^2/c^2)})t, \qquad (3)$$

which gives a slowing during the time of motion twice that of the Lorentz transformation (1).

But even then, the interpretation as a physical effect seems to me impossible, because the slowing depends upon an arbitrary choice of inertial reference frame of the stationary clock, and which therefore cannot be uniquely determined. That is, an arbitrary number of inertial reference frames different from the moving clock would subject the clock to an arbitrary number of different slowing effects at the same time, or if we limit the effect to one stationary reference frame, then by simply choosing either of two different stationary reference frames we would produce two different results.

The experimental evidence claiming to support this second interpretation can be divided into two types. The first measures the clock during the time of motion. In this case, if the observed time difference appears to be consistent with the Lorentz transformation, then the experiment would, according to the above argument, support the first interpretation, but not the second. Therefore this type of experiment need not be examined.

The second type of experiment is one where the moving clock is brought to rest and compared with the stationary clock, the elapsed time interval of motion compared, so that only a physical change over the time of travel would be observed. The results claimed by [2] are based on the behavior of synchronized cesium clocks on the Earth's surface and in aircraft flying in opposite directions with respect to the Earth's rotation, and then returning to the point of departure.

The elapsed times of the different clocks over the time of travel were compared with the predicted effect from the Lorentz transformation using

the Earth's axis as the stationary reference frame. Clocks flown in planes going in one direction showed a slower rate of time measure during the motion than the earth-bound clock, and those in the planes flying the opposite direction showed an increased rate. The experiment was criticized by [3,4] and was claimed to have been confirmed by [5].

I find the results interesting, as none of the issues discussed here are mentioned. In particular no reason is given why the clocks experienced the effects from the particular choice of stationary reference frame of the Earth's axis, but not from some other, in which case the clocks would have shown different results. An obvious choice would be the reference frame of the ground-based clock, that of the first example given by Einstein. In that case, both traveling clocks would have shown a slowing with respect to the ground-based clock.

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[3] A. G. Kelly, "Reliability of Relativistic Effect Tests on Airborne Clocks", Inst. Engineers Ireland Monograph No. 3 (February 1996)
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SANTILLI'S LIE-ADMISSIBLE MECHANICS. THE ONLY OPTION COMMENSURATE WITH IRREVERSIBILITY AND NONEQUILIBRIUM THERMODYNAMICS[1]

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Abstract

Our analysis of time reversal symmetry of various dynamical equations of fluid dynamics including Boltzmann integro-differential equation reveals that in a good number of cases there are no unique methods to relegate them to the so-called irreversible category unambiguously though they neither can be grouped into the reversible category. This substantiates Professor Santilli's No Reduction Theorem [1–3] that formed a base to develop genomathematics [4]. Hence, we once again substantiate the assertion of Professor Santilli that the only option commensurate with irreversibility and nonequilibrium thermodynamics is Santilli's Lie-Admissible Mechanics.

Keywords: Time reversal symmetry, Genomathematics, Lie Admissibility, Thermodynamics, Irreversible Thermodynamics, Irreversibility, Kinetic Theory.

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1 Introduction

The real and virtual motions are described by mathematical equations. Traditionally there are two different ways to analyze whether they are reversible or irreversible descriptions. The dynamical irreversibility is determined and understood using a yard stick of time reversal symmetry. The second yard stick of irreversibility originates from the second law of thermodynamics (see for example: [5]) and also via Boltzmann integro-differential equation [6].

Indeed, the dynamical reversibility and irreversibility can be worked out in principle both at microscopic and macroscopic levels of considerations. Whereas the thermodynamic reversibility and irreversibility are determined at the macroscopic level only. It is believed that the reversibility and irreversibility aspects of mathematical descriptions are well understood using the 20^{th} century mathematics and they are sound too. However, Santilli has already illustrated and stressed the existing lacuna in them. However, we are elaborating in this presentation a few more existing ambiguities in case we still continue with the 20^{th} century mathematics and physics.

For instance, one striking example is that of the following unresolved paradox, the Loschmidt paradox (J. Loschmidt, *Sitzungsber. Kais. Akad. Wiss. Wien, Math. Naturwiss.* Classe 73, 128 -142 (1876)).

Consider the case of a non-uniform dilute monatomic gas. Its molecules follow the reversible dynamics, that is *these molecules follow the invariant to time reversal Newtonian equations.* But when the time variation of Boltzmann-H function is computed, which involves the kinetic theory based averaging for all molecules over all velocities, the *result is its negative definite time rate.* This is the well known *Boltzmann H-theorem.*

That is the *bi-directional dynamics* of individual molecules produces *unidirectional evolution* of the system. This computed behaviour with time of H-function is then juxtaposed with the law of monotonic increase of entropy of thermodynamics and then it is proposed that the Boltzmann constant times the negative of this H-function is equal to Clausius' entropy.

Notice that *this approach only side tracks the above paradox it is not at all its solution.*

The purpose of this presentation is to elaborate the ambiguities that result on applying the time reversal symmetry test to a good number of well

known dynamical equations from fluid dynamics, discuss thermodynamical and dynamical reversibility (irreversibility) and then conclude that all the existing shortcomings get resolved if one adopts the genomathematics based dynamics [7, 8].

2 Reversibility and irreversibility vis-à-vis time reversal symmetry

Let us begin with a brief review of the reversibility and irreversibility aspects both dynamical and thermodynamical ones.

2.1 Thermodynamic reversibility

A macroscopic system when in equilibrium possesses no fluxes and spatial gradients within and across its boundaries. These states are time independent. A path through a succession of equilibrium states is termed as thermodynamically reversible. The *thermodynamic reversibility* gets mathematically described as follows,

$$\begin{aligned}
(a) \qquad dS = \frac{dQ}{T} \quad &\Longrightarrow \quad (-dS) = \frac{(-dQ)}{T} \Longrightarrow dS = \frac{dQ}{T} \\
(b) \quad dU = dQ - p\,dV \quad &\Longrightarrow \quad (-dU) = (-dQ) - p\,(-dV) \\
&\Longrightarrow \quad dU = dQ - p\,dV \\
(c)\ dU = TdS - p\,dV \quad &\Longrightarrow \quad (-dU) = T(-dS) - p\,(-dV) \\
&\Longrightarrow \quad dU = TdS - p\,dV \qquad (1)
\end{aligned}$$

Notice that dQ is the differential amount of heat exchanged by the system in the forward direction and $(-dQ)$ is that in the reverse direction, but dQ is not a state function. Whereas when a system evolves in time it possesses in general fluxes, spatial gradients and velocity vector and they are the dynamic state determining candidates and obviously are time dependent functions.

Thus an equilibrium state of a closed system gets described by any two state functions out of the five offered by $dU = TdS - p\,dV$, namely

U, S, V, T, p but in this list obviously dQ doesn't appear. This is an *amazing outcome* that demonstrates the *tight hold of thermodynamic principles on the state of a system in equilibrium* (see for example: [5]). This result is well tested in laboratory.

In other words, a *thermodynamic reversible path* is the one on which a system can be equally carried along forward and reverse directions that guarantees the system to assume the identically same equilibrium states but in reverse order on reversing the transition. Hence on reversing the transition the magnitudes of heat and work exchanged by the system simply change their signs without altering their magnitudes. *Notice that this thermodynamic reversibility is not a result of the act of time reversal as there is no time parameter involved.*

2.2 Dynamic reversibility and irreversibility

On the other hand, *all the time dependent processes are irreversible.* This is so because the past times and past situations are unattainable. However, for such processes the traditionally derived mathematical descriptions are based on Newtonian and Hamiltonian mechanics. Obviously they involve time parameter. This then offers an opportunity to analyze them for their behaviour against the time reversal operation and see if past situations can be attained or not. Amazingly, this exercise produces both *reversible* and also overall *irreversible* results.

For example, Newtonian dynamics of a particle or a rigid body in motion reads as [9]:

$$m\frac{d\mathbf{u}}{dt} = \mathbf{F}, \quad \mathbf{v} = \mathbf{u} + (\mathbf{F}/m)t \tag{2}$$

where $\mathbf{u}$ and $\mathbf{v}$ are the velocities, $\mathbf{F}$ is the body force acting on the particle of mass m and t is time. Notice that eq.(2) when describes the forward motion say from state A to state B the same equation does describe the motion from B to A seemingly following the same trajectory in the reverse order. However, the forward motion and the said reverse motion both are irreversible in time and hence the corresponding equation needs to be irreversible in time. This property as such is not inherited in eq.(2).

Let us further illustrate it by an example. In practice if one throws

a stone vertically straight up, it travels through a succession of positions upward and while coming down it follows the same succession of heights and positions but in reverse order. Indeed, $\mathbf{v} = \mathbf{u} + \mathbf{f}\,t$ holds good both for a motion upward and downward. However, in the said upward motion the velocities have positive sign whereas during downward motion all velocities have negative sign. Hence, at each position the dynamical state is not identically same during upward and downward motions. Moreover, during downward motion time t never becomes $-t$ instead it still remains positive and increases continuously. Hence, in reality there is no time reversal at all. This gets better illustrated pictorially as follows.

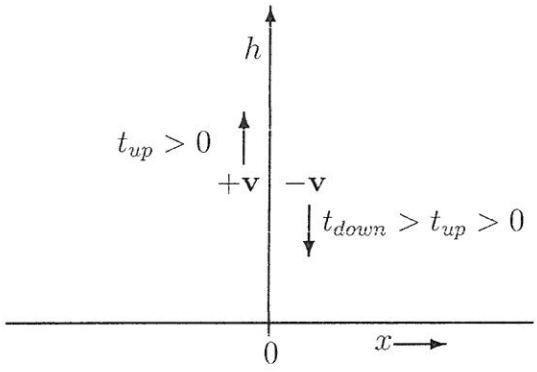

Figure 1: A schematic view of the upward and downward motion.

In Figures 1 and 2 we have represented the considered motion in two frames. The first one is in the spatial frame and the second one is in the time frame. Notice that Figure 2 clearly illustrates that even during downward motion of the particle – time increases. Thus though in the spatial representation the downward motion appears as a backward motion but in the time frame it is indeed a forward motion as there is no time reversal. In other words, *there is seemingly spatial reversibility of motion because time and velocity reversal have been ignored.* Of course, the motion is described throughout by one and the same equation $\mathbf{v} = \mathbf{u} + \mathbf{f}\,t$.

Thus the downward motion is not a reverse motion in true sense because going up and coming down constitutes one single forward motion.

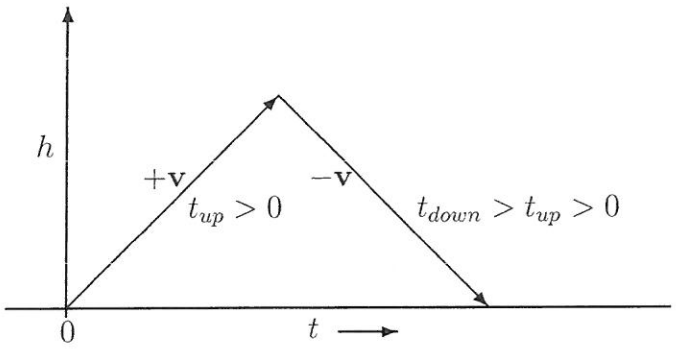

Figure 2: A schematic view of the upward and downward motion in time frame.

The reversibility of Newtonian equation say, $\mathbf{v} = \mathbf{u} + \mathbf{f}\,t$ (c.f. eq.(2)), where now $\mathbf{f}$ is the per unit mass force ($= \mathbf{F}/m$), is traditionally described as follows. It is the determination of time reversal symmetry just by substituting $-t$ for t that reverses the sign of velocities,

$$\mathbf{u} = \frac{d\mathbf{r}}{dt} \xrightarrow{t \to -t} \frac{d\mathbf{r}}{d(-t)} = -\mathbf{u}. \tag{3}$$

Hence one is led to,

$$\mathbf{v} = \mathbf{u} + \mathbf{f}\,t \overset{T}{\Longrightarrow} -\mathbf{v} = -\mathbf{u} + \mathbf{f}\,(-t) \longrightarrow \mathbf{v} = \mathbf{u} + \mathbf{f}\,t \tag{4}$$

where the transformation $(\mathbf{r},\, \mathbf{u},\, t) \to (\mathbf{r},\, -\mathbf{u},\, -t)$ has been symbolically represented by $\overset{T}{\Longrightarrow}$.

Now let us consider also the act of time reversal and its outcome. For the sake of demonstration let us effect time reversal after the particle has attained a certain height say h_1 at that moment the time elapsed is say t_1. In standard terminology the motion gets reversed but it would be a virtual motion not the real one. This gets depicted in time frame as shown

in Figure 3.

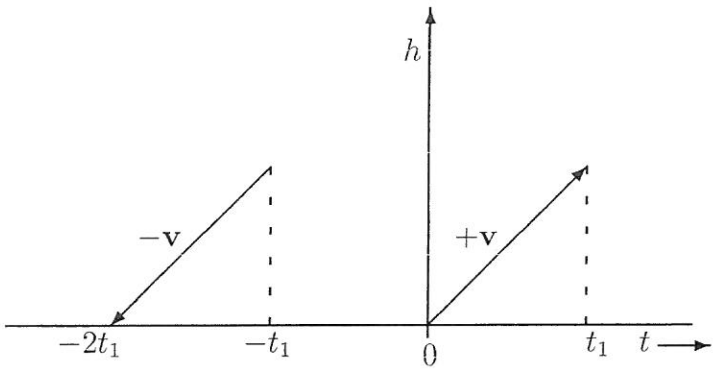

Figure 3: A schematic view of the dynamics on the act of time reversal.

Thus we see that the instantaneous time reversal puts the motion in different time-space and hence the forward and the time reversed motions do not coincide. The two trajectories would coincide only if simultaneously the zero of time is shifted to t_1. But this is not implied by $\stackrel{T}{\Longrightarrow}$. However, even if we include shifting of zero of time in $\stackrel{T}{\Longrightarrow}$, the dynamic state still remains different because instead of $\mathbf{v}$ there we have $-\mathbf{v}$ on the time reversed trajectory. From the above discussion it is clear that every time dependent motion is, in actuality, *irreversible* in time frame. However, traditionally we describe all real motions using equations and they are symmetric to time reversal operation. In other words, we are using time reversible equations to describe irreversible motions. Thus incompatible mathematical equations are being used.

On the other hand, as described above the time reversal operation $\stackrel{T}{\Longrightarrow}$ can be executed at any stage of the motion and its result would be the reversal of motion both in space and in time. However, this is a paper and pencil operation because for the observer time is still increasing. Or in other words, *the time reversed motion is an imaginary motion.* That is, *the time reversal operation is not a physical reality.* However, the time

reversal operation seemingly gives an opportunity to *visualize past situations* without actually going into the past as going into the past is impossible. This is so because as discussed above the past dynamic states are never achieved by time reversal.

Moreover, we will see below that there is *a large number of dynamic situations whose traditional mathematical descriptions when subjected to the time reversal operation produces ambiguous results.* This then questions the *very basis of time reversal operation from its physical utility point of view.*

Precisely the above fundamental facts led Professor R. M. Santilli to discover suitable mathematics. Following decades of systematic and sustained research Santilli [1] has achieved a *genotopic* (that is, axiom inducing) lifting of 20^{th} century mathematics with a Lie algebra structure as used for reversible systems into a *covering Lie-admissible form which is irreversible* beginning with the basic multiplications and related units, today is known as *Santilli genomathematics.*

Besides this, he achieved an isotopic (that is, axiom-preserving) lifting of 20^{th} century Lie mathematics with a Lie-isotopic structure, today known as *Santilli's isomathematics.* Finally, Santilli has discovered an anti-Hermitean map, called *isoduality*, for the description of antimatter, resulting in the novel *isodual genomathematics* and *isodual isomathematics*, that have permitted the first known initiation of thermodynamical studies of antimatter. Moreover, one of the fundamental and striking discoveries of Santilli is the **No Reduction Theorem** [3] that reads as,

> *A classical system that is irreversible over time cannot be consistently reduced to a finite number of elementary particles all reversible over time and, vice-versa, a finite number of elementary particles all in reversible conditions cannot yield a macroscopic irreversible event under the correspondence or other principles.*

The above theorem has far reaching implications on *bridging macroscopic and microscopic domains of physical descriptions.* Santilli's new mathematics removed almost all inadequacies of all branches of physics, which were so far presented using 20^{th} century mathematics and mechanics. Hence, it is no exaggeration to state that now we have *New Sciences for A New Era.*

2.3 Thermodynamic irreversibility

The origin of the description of thermodynamic irreversibility lies in the second law of thermodynamics, which inherently is based on the *global level of considerations.* It is stated as follows. *The entropy of a system can change on two and only two counts. The one is by the exchange of entropy, which can be positive or negative and the second is by the production of entropy, which is positive definite.* For a closed system it is mathematically stated as [10]:

$$\frac{dS}{dt} = \frac{d_eS}{dt} + \frac{d_iS}{dt}, \quad \frac{d_eS}{dt} \gtreqless 0, \quad \frac{d_iS}{dt} \geq 0$$

where S is the entropy of the system, $\dfrac{d_eS}{dt}$ is the rate of exchange of entropy which can be positive or negative and $\dfrac{d_iS}{dt}$ is the rate of entropy production which is always positive definite. Whereas in the case of a non-uniform system it is stated at *local level* as *Clausius-Duhem inequality* [11, 12], namely:

$$\rho\frac{ds}{dt} + \nabla \cdot \mathbf{J}_s = \sigma_s \geq 0$$

where s is per unit mass entropy, $\mathbf{J}_s$ is the entropy flux density and σ_s is the entropy source strength.

1. The existence of $\mathbf{J}_s$ and σ_s at the local level implies the *existence of thermodynamic irreversibility.*

2. However, for the *existence of thermodynamic irreversibility* the non-zero and positive definite σ_s at the local level or $\dfrac{d_iS}{dt}$ at the global level is the necessary and sufficient requirement. This is so because for an adiabatically closed system $\dfrac{d_eS}{dt} = 0$ that does'nt mean that $\dfrac{d_iS}{dt} = 0$. Similarly, if there is no temperature gradient within the system we have $\mathbf{J}_s = 0$ but σ_s could be non-zero. Also in a nonequilibrium stationary state we have at each interior point $\nabla \cdot \mathbf{J}_s = 0$ but σ_s remains non-zero.

This is the thermodynamic description of irreversibility. As we are analyzing the practical utility of time reversal symmetry let us see how the above thermodynamic expressions and equations behave on the time reversal operation.

1. We recall that at every stage of evolution of the system *the second law of thermodynamics guarantees the non-zero and positive definite values of* σ_s *at the local level and positive definite non-zero value of* $\frac{d_i S}{dt}$ *at the global level.*

2. It, therefore, means that *even at a past stage of evolution* of a thermodynamic system σ_s and $\frac{d_i S}{dt}$ *were positive definite.*

3. Hence, *if the time reversal implies leading us to past times and corresponding situations* then σ_s and $\frac{d_i S}{dt}$ *cannot change their sign.*

4. That is, σ_s and $\frac{d_i S}{dt}$ should *remain time reversal invariant.* But this result is not provided by the time reversal operation but in combination with the requirement of the second law of thermodynamics we have,

$$\frac{dS}{dt} = \frac{d_e S}{dt} + \frac{d_i S}{dt} \stackrel{T}{\Longrightarrow} -\frac{dS}{dt} = -\frac{d_e S}{dt} + \frac{d_i S}{dt}$$

$$\rho \frac{ds}{dt} + \nabla \cdot \mathbf{J}_s = \sigma_s \stackrel{T}{\Longrightarrow} -\rho \frac{ds}{dt} - \nabla \cdot \mathbf{J}_s = \sigma_s$$

5. Because the entropy flux $\mathbf{J}_s$ changes its sign on time reversal it implies that the time reversed path so obtained is not identically the same one that was traversed in forward direction.

6. Thus attaining of the past states through time reversal is not achieved even though the entropy production and entropy source strength have been assumed to retain their signs as per the demand of the second law of thermodynamics.

7. Thus we see that the *dynamic irreversibility demonstrated by time reversal operation of entropy balance equations* is the result of *thermodynamic irreversibility* (invariance of entropy production term on time reversal) guaranteed by the second law of thermodynamics and not as a result of the time reversal operation.

To have a better understanding of time reversal symmetry vis-à-vis nonequilibrium thermodynamic descriptions let us go a little more in deep. First we recall that at a *nonequilibrium stationary state* (NSS) ($dS/dt = 0$ and $\rho ds/dt = 0$) from the corresponding above two equations we have,

$$-\frac{d_e S}{dt} = \frac{d_i S}{dt} = \text{constant} > 0$$

and

$$\nabla \cdot \mathbf{J}_s = \sigma_s = \text{constant} > 0$$

That is there we have non-zero positive definite values of σ_s at the local level and $\frac{d_i S}{dt}$ at the global level. Thus as *a NSS is the time independent state one should not apply the time reversal operation on equation describing it* although the entropy is being produced and entirely exchanged out at a constant rate.

Let us examine the standard nonequilibrium thermodynamic expressions of entropy production and entropy exchange. In classical irreversible thermodynamics (CIT) [13] we have the following equation of entropy balance,

$$\begin{aligned}\rho\frac{ds}{dt} &= -\nabla\cdot\left(\frac{\mathbf{q}-\sum_k \mu_k\mathbf{J}_k}{T}\right) + \mathbf{q}\cdot\nabla\left(\frac{1}{T}\right) + T^{-1}\boldsymbol{\Pi} : \nabla\mathbf{u} \\ &\quad -\frac{1}{T}\sum_k \mathbf{J}_k\cdot\left(T\,\nabla\left(\frac{\mu_k}{T}\right) - \mathbf{F}_k\right) + \sum_\gamma \frac{\mathcal{A}^\gamma}{T}\frac{d\xi^\gamma}{dt}\end{aligned}$$

where the entropy flux, $\mathbf{J}_s$, and entropy source strength, σ_s in this case are given by,

$$\mathbf{J}_s = \left(\frac{\mathbf{q} - \sum_k \mu_k \mathbf{J}_k}{T} \right) \gtrless 0$$

$$\begin{aligned} \sigma_s &= \mathbf{q} \cdot \nabla \left(\frac{1}{T} \right) + T^{-1} \mathbf{\Pi} : \nabla \mathbf{u} \\ &\quad - \frac{1}{T} \sum_k \mathbf{J}_k \cdot \left(T \nabla \left(\frac{\mu_k}{T} \right) - \mathbf{F}_k \right) + \sum_\gamma \frac{\mathcal{A}^\gamma}{T} \frac{d\xi^\gamma}{dt} \geq 0 \end{aligned}$$

On time reversal, for example, we will have,

$$\begin{aligned} -\rho \frac{ds}{dt} &= +\nabla \cdot \left(\frac{\mathbf{q} - \sum_k \mu_k \mathbf{J}_k}{T} \right) - \mathbf{q} \cdot \nabla \left(\frac{1}{T} \right) + T^{-1} \mathbf{\Pi} : \nabla \mathbf{u} \\ &\quad + \frac{1}{T} \sum_k \mathbf{J}_k \cdot \left(T \nabla \left(\frac{\mu_k}{T} \right) - \mathbf{F}_k \right) + \sum_\gamma \frac{\mathcal{A}^\gamma}{T} \frac{d\xi^\gamma}{dt} \end{aligned}$$

From above expressions the expression after time reversal operation of the entropy flux density, $\mathbf{J}'_s$, and entropy source strength, σ'_s are obtained as,

$$\mathbf{J}'_s = -\mathbf{J}_s = - \left(\frac{\mathbf{q} - \sum_k \mu_k \mathbf{J}_k}{T} \right) \gtrless 0$$

$$\begin{aligned} \sigma'_s &= -\mathbf{q} \cdot \nabla \left(\frac{1}{T} \right) + T^{-1} \mathbf{\Pi} : \nabla \mathbf{u} \\ &\quad + \frac{1}{T} \sum_k \mathbf{J}_k \cdot \left(T \nabla \left(\frac{\mu_k}{T} \right) - \mathbf{F}_k \right) + \sum_\gamma \frac{\mathcal{A}^\gamma}{T} \frac{d\xi^\gamma}{dt} \neq \sigma_s \end{aligned}$$

From above we see that the entropy flux density reverses its sign on time reversal. On the other hand, in the case of entropy source strength we see that on time reversal except viscous dissipation and chemical reaction terms all terms are assumed to reverse their sign. Of course, we could have assumed invariance of $\mathbf{\Pi}$ on time reversal on considering it as comprised by the components of the contact forces. Thus it leads to reversing of the sign of corresponding contribution to entropy source strength, but that contradicts the second law of thermodynamics.

Let us also consider why we have time reversal invariance of the chemical reaction term. This we illustrate by considering that within the system only a single chemical reaction proceeds at a finite rate. For the sake of demonstration we consider a chemical reaction $A \underset{k_b}{\overset{k_f}{\rightleftharpoons}} B$ with k_f and k_b being the forward and backward rate constants and A and B are the reactant and the product respectively. For this chemical reaction the chemical affinity $\mathcal{A}$ reads as [13],

$$\mathcal{A} = \mu_A - \mu_B$$

where μ_A and μ_B are the respective chemical potentials, and the rate of chemical reaction, $\dfrac{d\xi}{dt}$, based on the law of mass action is given by (see for example: [14],

$$\frac{d\xi}{dt} = k_f C_A - k_b C_B$$

where C_A and C_B are the instantaneous concentrations of A and B.

Now on time reversal none of the terms μ_A, μ_B, k_f, k_b, C_A and C_B change their sign nor can instantly change their numerical values. Hence on time reversal neither $\mathcal{A}$ nor $\dfrac{d\xi}{dt}$ change their sign. Hence chemical reaction doesn't get reversed on time reversal. This explains how second law of thermodynamics remains valid in this case even after time reversal.

Perhaps, the same behaviour should have been shown by the other terms of entropy source strength that originate from spatial non-uniformity. This difference in behaviour suggests that *CIT has erred in admitting spatial non-uniformity in the domain of the applicability of Gibbs relation*, which has been postulated as a prescription of local equilibrium. The present author has already pointed out earlier this error in the postulation of local

equilibrium through the adoption of Gibbs relation in time rate form [8,15–20] to develop CIT. However, CIT given entropy source strength expressions for spatial non-uniformity have been well tested in laboratory for various nonequilibrium stationary states (e.g. Ficks law of diffusion, Ohm's law, Navier-Stokes relations, electro-kinetic effects, electro-mechanical effects, thermo-diffusion effects, etc.) and hence if we exclude the irreversibility on account of chemical reactions then the CIT given description turns out valid only for NSS [8, 19, 20].

On the other hand, in extended irreversible thermodynamics (EIT) [21] corresponding expression of σ_s to the first approximation (in absence of body forces and assuming Maxwell- Cattaneo-Vernotte (MCV) type of constitutive equations [22, 23] for diffusion fluxes) is,

$$\sigma_s = \beta_{\mathbf{q}}\mathbf{q}\cdot\mathbf{q} + \beta_{\mathbf{\Pi}}\mathbf{\Pi}:\mathbf{\Pi} + \sum_k \beta_{\mathbf{J}_k}\mathbf{J}_k\cdot\mathbf{J}_k + \sum_\gamma \frac{\mathcal{A}^\gamma}{T}\frac{d\xi^\gamma}{dt} \geq 0$$

Thus we see that on time reversal, irrespective of fluxes change their sign or not, the first three terms on the right hand side of entropy source strength do not change their sign. Also as demonstrated above the chemical reaction term is time reversal invariant. Hence, if we use EIT expression of entropy source strength the second law of thermodynamics is not flouted on the time reversed path.

2.4 Boltzmann equation, Boltzmann's H-theorem and macroscopic irreversibility

The Boltzmann integro-differential equation for monatomic gas on neglecting body forces reads as [24],

$$\frac{\partial f}{\partial t} + \mathbf{c}\cdot\frac{\partial f}{\partial \mathbf{r}} = J(f|f)$$

where f is the distribution function corresponding to the molecular velocity $\mathbf{c}$, $\mathbf{r}$ is the position vector and $J(f|f)$ is the Boltzmann collisional integral given by:

$$J(f|f) = \int\int (f_1' f' - f_1 f) g\sigma(g,\Omega) d\Omega d\mathbf{c}_1$$

where $\sigma(g,\Omega)$ is the collision cross section that depends on the relative velocity $g = |\mathbf{c}_1 - \mathbf{c}|$ and the scattering solid angle Ω. The primes and indices in the distribution function have the usual meaning, namely, $f_1' = f(\mathbf{c}_1', \mathbf{r}, t)$ is the distribution function of particle 1 after collision, etc.

The left hand side of the Boltzmann equation changes sign on time reversal operation, namely:

$$\frac{\partial f}{\partial t} + \mathbf{c}\cdot\frac{\partial f}{\partial \mathbf{r}} \overset{T}{\Longrightarrow} \frac{\partial f}{\partial(-t)} + (-\mathbf{c})\cdot\frac{\partial f}{\partial \mathbf{r}} \Rightarrow -\left(\frac{\partial f}{\partial t} + \mathbf{c}\cdot\frac{\partial f}{\partial \mathbf{r}}\right)$$

but the right hand side of Boltzmann equation is obtained as time reversal invariant, namely:

$$J(f|f) = \int\int (f_1'f' - f_1 f) g\sigma(g,\Omega) d\Omega d\mathbf{c}_1 \overset{T}{\Longrightarrow}$$
$$J(f|f) = \int\int (f_1'f' - f_1 f) g\sigma(g,\Omega) d\Omega d\mathbf{c}_1$$

because it does not contain t explicitly. *Thus it appears that the Boltzmann integro-differential equation is obtained as antisymmetric to the operation of time reversal.*

So far so good but let us analyze it further. On instantaneous time reversal all molecules would reverse their motion then the distribution functions before collision should become those of after collision and vice versa. Then we would have $(f_1'f' - f_1 f) \overset{T}{\Longrightarrow} (f_1 f - f_1'f') \Rightarrow -(f_1'f' - f_1 f)$. However, the effecting of this time reversal operation does imply $f(\mathbf{c}, \mathbf{r}, t) = f(-\mathbf{c}, \mathbf{r}, -t)$. With this insight the *Boltzmann equation is obtained as time reversal invariant.*

But in essence the time reversal operation means the substitution of $-t$ for t without any alteration in the equation. Thus we see that both the options of time reversal operation have their own shortcomings. With these two options for time reversal symmetry of Boltzmann integro-differential equation, now let us examine the famous Boltzmann's H-theoem.

Boltzmann defined kinetic theory based H-function [6] whose negative

is the kinetic theory definition of entropy function[3]. It reads as,

$$\rho\, s = -k_B \int f(\ln f - 1) d\mathbf{c}$$

where k_B is the Boltzmann constant.

On differentiation of above equation with respect to time and further effecting the standard mathematical manipulations produces,

$$\frac{\partial \rho s}{\partial t} = -div\,(\rho s \mathbf{u} + \mathbf{J}_s) + \sigma_s$$

where the entropy flux density, $\mathbf{J}_s$, is given by,

$$\mathbf{J}_s = -k_B \int \mathbf{C} f\,(\ln f - 1)\, d\mathbf{c}$$

where $\mathbf{C}$ is the molecular peculiar or chaotic velocity, and the entropy source strength, σ_s, is given by,

$$\sigma_s = -k_B \int J(f|f) \ln f d\mathbf{c}$$

The entropy source strength, σ_s, is further mathematically manipulated to produce,

$$\sigma_s = \frac{1}{4} k_B \int\int\int \left(\ln \frac{f' f_1'}{f f_1}\right) (f_1' f' - f_1 f)\, g^3 \sigma(g,\, \Omega) d\Omega d\Omega' dg d\mathbf{c}_{(1)} \geq 0$$

where $\mathbf{c}_{(1)}$ is the center of mass velocity of the colliding molecular pair. The positive definiteness shown in the preceding equation stems from the fact that if $\ln \frac{f' f_1'}{f f_1} > 0$ then we have $(f_1' f' - f_1 f) > 0$ and if the former is < 0 then the latter is also < 0 the rest of the terms of the integrands are positive numbers by definition. This is the *Boltzmann's H-theorem* [13].

---

[3]Actually the H-function has been defined by Boltzmann as,

$$H = \int f \ln f d\mathbf{c}$$

which was later found to relate with the entropy function given in the main text.

Now we see that the positive definiteness of the preceding equation is time reversal invariant in both the above stated options of change or no change of the roles of the distribution functions on time reversal operation. This is a *paradoxical* situation because *irrespective of the Boltzmann equation is taken time reversal invariant or variant the H-theorem that results from it is obtained as time reversal invariant.* Therefore, in literature it is taken as the kinetic theory version of second law of thermodynamics [13].

3 Time reversal symmetry of dynamical equations

Notice that we have used in introduction only an elementary equation of Newtonian mechanics to illustrate the incompatibility of it with the observed irreversibility in time frame. Of course, that discussion is adequate in illustrating the incompatibility 20^{th}-century mathematics to describe irreversibility. However, it is worth considering what other inconsistencies and ambiguities are encountered when we subject the conventional fluid dynamical equations to the time reversal operation. Let us illustrate it systematically.

3.1 Determination of time reversal symmetry. Simple Equations

Let us first apply the above test to certain basic equations from fluid dynamics [9, 13] which are obtained as symmetric to the time reversal operation.

Relation between **convective and local time derivatives**:

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla \overset{T}{\Longrightarrow} \frac{d}{d(-t)} = \frac{\partial}{\partial(-t)} + (-\mathbf{u})\cdot\nabla$$
$$\Rightarrow \frac{d}{dt} = \frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla$$

Relation between **convective and local time derivatives of mass den-**

sity, ρ:

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \nabla \rho \overset{T}{\Longrightarrow} \frac{d\rho}{d(-t)} = \frac{\partial \rho}{\partial(-t)} + (-\mathbf{u}) \cdot \nabla \rho$$
$$\Rightarrow \frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \nabla \rho$$

Relation between **convective and local time derivatives of velocity vector, u** :

$$\frac{d\mathbf{u}}{dt} = \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \overset{T}{\Longrightarrow} \frac{d(-\mathbf{u})}{d(-t)} = \frac{\partial(-\mathbf{u})}{\partial(-t)} + (-\mathbf{u}) \cdot \nabla(-\mathbf{u})$$
$$\Rightarrow \frac{d\mathbf{u}}{dt} = \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}$$

Eulerian equation of continuity:

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{u}) \overset{T}{\Longrightarrow} \frac{\partial \rho}{\partial(-t)} = -\nabla \cdot (\rho(-\mathbf{u}))$$
$$\Rightarrow \frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{u})$$

Lagrangian equation of continuity:

$$\frac{d\rho}{dt} = -\rho \nabla \cdot \mathbf{u} \overset{T}{\Longrightarrow} \frac{d\rho}{d(-t)} = -\rho \nabla \cdot (-\mathbf{u})$$
$$\Rightarrow \frac{d\rho}{dt} = -\rho \nabla \cdot \mathbf{u}$$

Lagrangian equation of continuity in terms of specific volume, $v = \rho^{-1}$:

$$\rho \frac{dv}{dt} = \nabla \cdot \mathbf{u} \overset{T}{\Longrightarrow} \rho \frac{dv}{d(-t)} = \nabla \cdot (-\mathbf{u})$$
$$\Rightarrow \rho \frac{dv}{dt} = \nabla \cdot \mathbf{u}$$

Relation between Lagrangian and Eulerian dynamics of a property:

$$\rho\frac{dz}{dt} = \frac{\partial \rho z}{\partial t} + \nabla\cdot(\rho z\mathbf{u}) \overset{T}{\Longrightarrow} \rho\frac{dz}{d(-t)} = \frac{\partial \rho z}{\partial(-t)} + \nabla\cdot(\rho z(-\mathbf{u}))$$
$$\Rightarrow \rho\frac{dz}{dt} = \frac{\partial \rho z}{\partial t} + \nabla\cdot(\rho z\mathbf{u})$$

where z is a per unit mass quantity.

Now assume that only the conservative body forces act upon a *rigid body in motion*, that means:

$$\mathbf{F} = -\nabla\psi, \quad \frac{\partial \psi}{\partial t} = 0, \quad \frac{\partial \mathbf{F}}{\partial t} = 0$$

Equation of motion in Eulerian form:

$$\frac{\partial \rho\mathbf{u}}{\partial t} = -\nabla\cdot(\rho\mathbf{u}\mathbf{u}) + \rho\,\mathbf{F}$$
$$\overset{T}{\Longrightarrow} \frac{\partial \rho(-\mathbf{u})}{\partial(-t)} = -\nabla\cdot(\rho(-\mathbf{u})(-\mathbf{u})) + \rho\,\mathbf{F}$$
$$\Rightarrow \frac{\partial \rho\mathbf{u}}{\partial t} = -\nabla\cdot(\rho\mathbf{u}\mathbf{u}) + \rho\,\mathbf{F}$$

Equation of motion in Lagrangian form:

$$\rho\frac{d\mathbf{u}}{dt} = \rho\mathbf{F} \overset{T}{\Longrightarrow} \rho\frac{d(-\mathbf{u})}{d(-t)} = \rho\mathbf{F}$$
$$\Rightarrow \rho\frac{d\mathbf{u}}{dt} = \rho\mathbf{F}$$

Kinetic energy balance equation in Eulerian form:

$$\frac{\partial \frac{1}{2}\rho\mathbf{u}^2}{\partial t} = -\nabla\cdot\left(\frac{1}{2}\rho\mathbf{u}^2\mathbf{u}\right) + \rho\,\mathbf{F}\cdot\mathbf{u}$$
$$\overset{T}{\Longrightarrow} \frac{\partial \frac{1}{2}\rho\mathbf{u}^2}{\partial(-t)} = -\nabla\cdot\left(\frac{1}{2}\rho\mathbf{u}^2(-\mathbf{u})\right) + \rho\,\mathbf{F}\cdot(-\mathbf{u})$$
$$\Rightarrow \frac{\partial \frac{1}{2}\rho\mathbf{u}^2}{\partial t} = -\nabla\cdot\left(\frac{1}{2}\rho\mathbf{u}^2\mathbf{u}\right) + \rho\,\mathbf{F}\cdot\mathbf{u}$$

Kinetic energy in Lagrangian form:

$$\rho\frac{d\frac{1}{2}\mathbf{u}^2}{dt} = \rho\,\mathbf{F}\cdot\mathbf{u} \quad \overset{T}{\Longrightarrow} \quad \rho\frac{d\frac{1}{2}\mathbf{u}^2}{d(-t)} = \rho\,\mathbf{F}\cdot(-\mathbf{u})$$
$$\Rightarrow \rho\frac{d\frac{1}{2}\mathbf{u}^2}{dt} = \rho\,\mathbf{F}\cdot\mathbf{u}$$

Potential energy in Eulerian form:

$$\frac{\partial\rho\psi}{\partial t} = -\nabla\cdot(\rho\psi\mathbf{u}) - \rho\,\mathbf{F}\cdot\mathbf{u}$$
$$\overset{T}{\Longrightarrow} \quad \frac{\partial\rho\psi}{\partial(-t)} = -\nabla\cdot(\rho\psi(-\mathbf{u})) - \rho\,\mathbf{F}\cdot(-\mathbf{u})$$
$$\Rightarrow \frac{\partial\rho\psi}{\partial t} = -\nabla\cdot(\rho\psi\mathbf{u}) - \rho\,\mathbf{F}\cdot\mathbf{u}$$

Potential energy in Lagrangian form:

$$\rho\frac{d\psi}{dt} = -\rho\,\mathbf{F}\cdot\mathbf{u} \quad \overset{T}{\Longrightarrow} \quad \rho\frac{d\psi}{d(-t)} = -\rho\,\mathbf{F}\cdot(-\mathbf{u})$$
$$\Rightarrow \rho\frac{d\psi}{dt} = -\rho\,\mathbf{F}\cdot\mathbf{u}$$

Total mechanical energy in Eulerian form:

$$\frac{\partial\rho\left(\frac{1}{2}\mathbf{u}^2+\psi\right)}{\partial t} = -\nabla\cdot\left[\rho\left(\frac{1}{2}\mathbf{u}^2+\psi\right)\mathbf{u}\right]$$
$$\overset{T}{\Longrightarrow} \quad \frac{\partial\rho\left(\frac{1}{2}\mathbf{u}^2+\psi\right)}{\partial(-t)} = -\nabla\cdot\left[\rho\left(\frac{1}{2}\mathbf{u}^2+\psi\right)(-\mathbf{u})\right]$$
$$\Rightarrow \frac{\partial\rho\left(\frac{1}{2}\mathbf{u}^2+\psi\right)}{\partial t} = -\nabla\cdot\left[\rho\left(\frac{1}{2}\mathbf{u}^2+\psi\right)\mathbf{u}\right]$$

Total mechanical energy in Lagrangian form:

$$\rho\frac{d\left(\frac{1}{2}\mathbf{u}^2+\psi\right)}{dt} = 0$$

All the *above equations are seen as time reversal symmetric* but as said above the question still remains that of its physical utility. Now in the next subsection we will examine more involved fluid dynamical equation for time reversal symmetry and we would see that it produces *ambiguous results.*

3.2 Equations producing ambiguous results

3.2.1 Rigid body motion

Total energy, e (per unit mass), in Eulerian form:

$$\frac{\partial \rho e}{\partial t} = -\nabla \cdot (\rho e \mathbf{u}) - \nabla \cdot \mathbf{J}_e$$
$$\stackrel{T}{\Longrightarrow} \frac{\partial \rho e}{\partial (-t)} = -\nabla \cdot (\rho e(-\mathbf{u})) - \nabla \cdot (-\mathbf{J}_e)$$
$$\Rightarrow \frac{\partial \rho e}{\partial t} = -\nabla \cdot (\rho e \mathbf{u}) - \nabla \cdot \mathbf{J}_e$$

Notice that the the conductive flux, $\mathbf{J}_e$, has been assumed to reverse its sign on time reversal as it is a flux.

However, we will see below while discussing corresponding internal energy balance equation that the time reversal symmetry or antisymmetry for the heat flux density is not an unambiguous choice and hence the same remains true of $\mathbf{J}_e$ as it is none else than the heat flux density.

Total energy in Lagrangian form:

$$\rho \frac{de}{dt} = -\nabla \cdot \mathbf{J}_e \stackrel{T}{\Longrightarrow} \rho \frac{de}{d(-t)} = -\nabla \cdot (-\mathbf{J}_e)$$
$$\Rightarrow \rho \frac{de}{dt} = -\nabla \cdot \mathbf{J}_e$$

The internal energy, u (per unit mass), is given by:

$$u = e - \left(\frac{1}{2}\mathbf{u}^2 + \psi \right)$$

Hence, **internal energy in Eulerian form** reads as:

$$\frac{\partial \rho u}{\partial t} = \frac{\partial \rho \left(e - \left(\frac{1}{2}\mathbf{u}^2 + \psi \right) \right)}{\partial t} = -\nabla \cdot (\rho u \mathbf{u} + \mathbf{J}_u)$$

where the convective flux of internal energy gets quantified as: $\rho u \mathbf{u} = \rho \left(e - \left(\frac{1}{2}\mathbf{u}^2 + \psi \right) \right) \mathbf{u}$ whereas in the present case there is no conductive flux of mechanical energy hence $\mathbf{J}_e = \mathbf{J}_u$.

Therefore, the time reversal operation produces,

$$\frac{\partial \rho u}{\partial t} = -\nabla \cdot (\rho u \mathbf{u} + \mathbf{J}_u) \overset{T}{\Longrightarrow} \frac{\partial \rho u}{\partial (-t)} = -\nabla \cdot (\rho u(-\mathbf{u}) + (-\mathbf{J}_u))$$
$$\Rightarrow \frac{\partial \rho u}{\partial t} = -\nabla \cdot (\rho u \mathbf{u} + \mathbf{J}_u)$$

Notice that $\mathbf{J}_u$ also has been assumed to change its sign on time reversal as it is none else but the $\mathbf{J}_e$ in the present case.

The **Lagrangian form of internal energy balance equation** in the present case reads as:

$$\rho \frac{du}{dt} = -\nabla \cdot \mathbf{J}_u = -\nabla \cdot \mathbf{q}$$

Thus $\mathbf{J}_u$ is nothing else but the heat flux density, $\mathbf{q}$.

Now we have,

$$\rho \frac{du}{dt} \overset{T}{\Longrightarrow} \rho \frac{du}{d(-t)} = -\rho \frac{du}{dt}$$
$$\text{it implies that:} \quad -\nabla \cdot \mathbf{q} \overset{T}{\Longrightarrow} -(-\nabla \cdot \mathbf{q})$$
$$\text{this can happen only when:} \quad \mathbf{q} \overset{T}{\Longrightarrow} -\mathbf{q}.$$

Moreover, in kinetic theory [6, 25, 26] the expression of heat flux is $\mathbf{q} = \overline{\rho \frac{1}{2} \mathbf{C}^2 \mathbf{C}}$ for a non-uniform monatomic gas, where $\mathbf{C}(= \mathbf{c} - \mathbf{u})$ is the chaotic velocity of a molecule and $\mathbf{c}$ is the molecular velocity. In view of this definition $\mathbf{C}$ would change its sign on time reversal as the sign of both $\mathbf{c}$ and $\mathbf{u}$ changes on time reversal. Therefore, $\mathbf{q} = \overline{\rho \frac{1}{2} \mathbf{C}^2 \mathbf{C}}$ would change it sign on time reversal.

This is mathematically illustrated below,

$$\mathbf{q} = \overline{\rho \frac{1}{2} \mathbf{C}^2 \mathbf{C}} \overset{T}{\Longrightarrow} \mathbf{q}' = \overline{\rho \frac{1}{2} (-\mathbf{C})^2 (-\mathbf{C})} = -\overline{\rho \frac{1}{2} \mathbf{C}^2 \mathbf{C}} = -\mathbf{q}$$

Thus $\mathbf{q}$ is obtained as time reversal antisymmetric. That is *on time reversed path heat flux has opposite sign.*

Now let us consider Maxwell-Cattaneo-Vernotte (MCV) equation [22, 23], namely:

$$\tau\frac{d\mathbf{q}}{dt}+\mathbf{q}=-\lambda\nabla T$$

where τ is the relaxation time and λ is the thermal conductivity. However, as heat flux reverses its direction on time reversal the MCV equation is obtained as not time invariant on time reversal, as shown below:

$$\tau\frac{d\mathbf{q}}{dt}+\mathbf{q}=-\lambda\nabla T \overset{T}{\Longrightarrow} \tau\frac{d(-\mathbf{q})}{d(-t)}+(-\mathbf{q})=-\lambda\nabla T$$
$$\Rightarrow \tau\frac{d\mathbf{q}}{dt}-\mathbf{q}=-\lambda\nabla T$$

However, the MCV equation may be considered a description that describes approach to corresponding nonequilibrium stationary state (NSS) and hence at NSS $\left(\frac{d\mathbf{q}}{dt}=0\right)$ MCV equation correctly produces the Fourier law, $\mathbf{q}=-\lambda\nabla T$.

While on the time reversed path we see from above that the Fourier law is not recovered if $\mathbf{q}$ has changed its sign. Therefore, *does it indicate that* $\mathbf{q}$ *is time reversal invariant*? Even if this is accepted the MCV equation is not obtained as time reversal invariant,

$$\tau\frac{d\mathbf{q}}{dt}+\mathbf{q}=-\lambda\nabla T \overset{T}{\Longrightarrow} \tau\frac{d(\mathbf{q})}{d(-t)}+(\mathbf{q})=-\lambda\nabla T$$
$$\Rightarrow -\tau\frac{d\mathbf{q}}{dt}+\mathbf{q}=-\lambda\nabla T$$

Furthermore, in CIT [13] the entropy source strength, σ_s, due to heat transfer is quantified as $\sigma_s=\mathbf{q}\cdot\nabla T^{-1}>0$. Thus if on time reversal $\mathbf{q}$ changes its sign then the second law of thermodynamics stands violated on the time reversed path. But if the above expression of entropy source strength corresponds to NSS then there is not need to apply time reversal

on it. Whereas, in extended irreversible thermodynamics (EIT) [21] we have $\sigma_s = \beta_{\mathbf{q}}\mathbf{q}^2 > 0$ hence even if $\mathbf{q}$ changes sign on time reversed path the second law is not violated.

From the above elaboration *one may perhaps assume that, in general* $\mathbf{q}$ *is not time reversal symmetric and hence the MCV equation is not time reversal symmetric.* But this is not the unambiguous option because as stated above *if we consider the corresponding expression of entropy source strength of CIT, on time reversal the second law of thermodynamics gets violated as heat flux changes its sign on time reversed path. Whereas in the case of EIT given expression of entropy source strength the time reversal does not violate the second law of thermodynamics.* Thus there does exist an ambiguity.

Now let us proceed to describe a few more fluid dynamical equations where no unambiguous conclusion about the time reversal symmetry can be made.

3.2.2 A viscous fluid in motion

In this case the *Eulerian form of momentum balance equation* is:

$$\frac{\partial \rho \mathbf{u}}{\partial t} = -\nabla \cdot (\rho \mathbf{u}\mathbf{u} - \mathcal{T}) + \rho\, \mathbf{F}$$

where $\mathcal{T}$ is the stress tensor, which measures the non-convective momentum flux density and alternately measures the normal and tangential forces per unit area. To be specific, the component, T_{ij}, of the stress tensor quantify the following:

$$\begin{aligned} T_{ij} &= (i - \text{component of force per unit area} \\ &\qquad \text{across a surface perpendicular to } \mathbf{e}_j) \\ &= (i - \text{component of momentum that crosses} \\ &\qquad \text{a unit area which is perpendicular to } \mathbf{e}_j, \text{per unit} \\ &\qquad \text{time, with the crossing being from } - x^j \text{ to } + x^j) \end{aligned}$$

The corresponding equation in Lagrangian form reads as:

$$\rho \frac{d\mathbf{u}}{dt} = \nabla \cdot \mathcal{T} + \rho\, \mathbf{F}$$

With the above physical explanations of $\mathcal{T}$ we are led to the following conclusions about its time reversal symmetry.

- Now as the components of $\mathcal{T}$ represent forces then on time reversal it should not change sign. Whereas its interpretation as a momentum flux suggests that it should change its sign on time reversal.
- In kinetic theory [6] we have $\mathcal{T} = \overline{\rho \mathbf{C}\mathbf{C}}$ hence as $\mathbf{C}$ changes sign on time reversal the sign of $\mathcal{T}$ would not change.

Thus we see that *there is no unambiguous way to decide the symmetry property of $\mathcal{T}$ on time reversal operation.*

In the premise of thermodynamics one uses fluid dynamical version of the first law of thermodynamics hence let us consider it,

$$\rho \frac{du}{dt} = -\nabla \cdot \mathbf{q} - p\rho \frac{dv}{dt} + \mathbf{\Pi} : \nabla \mathbf{u} + \sum_k \mathbf{J}_k \cdot \mathbf{F}_k$$

where $\mathbf{J}_k$ is the diffusion flux density of the component k and $\mathbf{F}_k$ is the body force per unit mass exerted on the chemical component k. Notice that on the right hand side of the preceding equation there is a term that contains $\mathbf{\Pi}$ in it, in view of the above discussion, the time reversal symmetry of the preceding equation remains ambiguous.

On the other hand, the first law of thermodynamics for spatially uniform systems in nonequilibrium reads as,

$$\frac{dU}{dt} = \frac{dQ}{dt} - p\frac{dV}{dt}$$

and it is seen that this equation is symmetric to time reversal (as dU, dQ, dV $\overset{T}{\Longrightarrow}$ $-dU$, $-dQ$, $-dV$ and $t \overset{T}{\Longrightarrow} -t$).

In view of the above illustration, *one would then use, in nonequilibrium thermodynamics, two different types of equations representing the first law of thermodynamics — one symmetric to time reversal and the other ambiguous on this count.* It would be then a bad commentary on thermodynamics.

3.3 Recapitulation and deductions

The above described elaborations unambiguously surface out the fact that on applying time reversal symmetry test to various fluid dynamical equations including the Boltzmann integro-differential equation we are led to the ambiguous results. Indeed, there is a distinction between *thermodynamic and dynamic reversibility* that is in the former case the identically same states are encountered on reversing the direction because the state of the system doesn't depend on the sign of the exchange differentials.

Whereas in the latter case *the direction of a vector associated with the system changes its sign hence seemingly traverses the same path in reverse direction. But as the dynamic state of a system is also determined by its associated vector, the time reversed paths consist of different dynamic states.* In view of this we recall the *no reduction theorem* of Santilli, namely *the reversible molecular dynamics cannot produce macroscopic irreversible description and vice-versa the irreversible macroscopic motion cannot be reduced to reversible molecular motion of its constituents* [1–3].

This then demands a mathematical apparatus inherited with unidirectionality of the description. *This demand is met by Santilli's genomathematics and the corresponding mechanics. In Santilli's genomathematics for forward and backward motions one uses different multiplying genounits* namely, for forward motion it is $\hat{I}^{>}$ and for the backward motion it is ${}^{<}\hat{I}$ and $\hat{I}^{>} \neq {}^{<}\hat{I}$. **It means that we have separate mathematical descriptions for forward and backward motions as they in reality are not reverse of each other.** That is *no time reversal symmetry test is required.*

Hence, we conclude that the **Santilli Lie-admissible mechanics** or **Santilli-Newtonian mechanics** [1, 3, 27] turns out as the *only option for mathematical description of irreversibility and hence for developing nonequilibrium thermodynamics too.*

For the sake of self-sufficiency in Section 4 we have described in brief Santilli's genomathematics and in Section 5 a few examples of genotopically lifted basic equations are given. This elaborates how Santilli's genomathematics when used to describe irreversible motions do not allow to creep-in the inconsistencies, ambiguities and confusions is described.

4 New mathematics

In geno-space there is no need to test time reversal symmetry of equations as in this setup all equations are generated as unidirectional in conformity with time's arrow associated with irreversible processes (see for example [4] and [28]). *My preliminary attempt as well as a short paper on Geno-GPITT* have recently appeared [29, 30].

4.1 Genomathematics

The main idea of genomathematics is the selection of *two different generalized units* called *genounits*,

- the first $\hat{I}^{>}$ for the *ordered multiplication to the right* $A > B$, called *forward genoproduct*, and
- the second ${}^{<}\hat{I}$ for the *ordered multiplication to the left* $A < B$, called *backward genoproduct*,

according to the general rules [31, 32]:

$$\hat{I}^{>} = 1/\hat{S},\ A > B = A \times \hat{S} \times B,\ \hat{I}^{>} > A = A > \hat{I}^{>} = A, \tag{5}$$

$${}^{<}\hat{I} = 1/\hat{R},\ A < B = A \times \hat{R} \times B,\ {}^{<}\hat{I} < A = A <^{<} \hat{I} = A, \tag{6}$$

where $\hat{S}$ and $\hat{R}$ are respective *genotopic elements*, that is for the forward and backward multiplications respectively.

$$A = A^{\dagger},\ B = B^{\dagger},\ \hat{R} = \hat{S}^{\dagger},\ \text{ and }\ \hat{R} \neq \hat{S} \tag{7}$$

hence we have by definition:

$$\hat{I}^{>} \neq {}^{<}\hat{I}$$

The *genounits* are conveniently generated from the isounit, $\hat{I}$, as follows,

$$\hat{I}^{>} = V \times \hat{I} \times V^{\dagger} > 0, \quad {}^{<}\hat{I} = W \times \hat{I} \times W^{\dagger} > 0 \tag{8}$$

Hence, we have,

$$\begin{aligned}\hat{S} &= (V \times \hat{I} \times V^{\dagger})^{-1} = V^{-1} \times \hat{I}^{-1} \times (V^{\dagger})^{-1} \\ &= V^{-1} \times \hat{T} \times (V^{\dagger})^{-1} = V^{-1} \hat{\times} (V^{\dagger})^{-1} > 0 \end{aligned} \tag{9}$$

Similarly,

$$\begin{aligned}\hat{R} &= (W \times \hat{I} \times W^{\dagger})^{-1} = W^{-1} \times \hat{I}^{-1} \times (W^{\dagger})^{-1} \\ &= W^{-1} \times \hat{T} \times (W^{\dagger})^{-1} = W^{-1} \hat{\times} (W^{\dagger})^{-1} > 0 \end{aligned} \tag{10}$$

That is we have opted,

$$V \times V^{\dagger} \neq 1, \quad W \times W^{\dagger} \neq 1$$

The *genotopic lifting* of *iso-multiplication of iso-numbers* get expressed as,

$$\begin{aligned}\hat{A} \hat{\times} \hat{B} \longrightarrow\ & V \times \left(\hat{A} \hat{\times} \hat{B} \right) \times V^{\dagger} \\ & = V \times \hat{A} \times \times V^{\dagger} \times (V^{\dagger})^{-1} \hat{\times} (V)^{-1} \times V \times \hat{B} \times \times V^{\dagger} \\ & = \hat{A}^{>} \times V^{-1} \times \hat{T} \times (V^{\dagger})^{-1} \times \hat{B}^{>} \\ & = \hat{A}^{>} \times \hat{S} \times \hat{B}^{>} = \hat{A}^{>} \hat{\times}^{>} \hat{B}^{>} \end{aligned} \tag{11}$$

and

$$\begin{aligned}\hat{A} \hat{\times} \hat{B} \longrightarrow\ & W \times \left(\hat{A} \hat{\times} \hat{B} \right) \times W^{\dagger} \\ & = W \times \hat{A} \times \times W^{\dagger} \times (W^{\dagger})^{-1} \hat{\times} (W)^{-1} \times W \times \hat{B} \times \times W^{\dagger} \\ & = {}^{<}\hat{A} \times W^{-1} \times \hat{T} \times (W^{\dagger})^{-1} \times {}^{<}\hat{B} \\ & = {}^{<}\hat{A} \times \hat{R} \times {}^{<}\hat{B} = {}^{<}\hat{A} \, {}^{<}\hat{\times} \, {}^{<}\hat{B} \end{aligned} \tag{12}$$

Thus we see that,

$$\hat{\times}^{>} = \times \hat{S} \times = \times V^{-1} \times \hat{T} \times (V^{\dagger})^{-1} \times \tag{13}$$

$${}^{<}\hat{\times} = \times \hat{R} \times = \times W^{-1} \times \hat{T} \times (W^{\dagger})^{-1} \times \tag{14}$$

The *genotopic lifting* of an *iso-quotient of iso-numbers* reads as,

$$\begin{aligned}\hat{A}\hat{\div}\hat{B} \quad \longrightarrow \quad & V\times(\hat{A}\hat{\div}\hat{B})\times V^{\dagger}=V\times\left(\frac{\hat{A}}{\hat{B}}\times\hat{I}\right)\times V^{\dagger}\\ &=\frac{V\times\hat{A}\times V^{\dagger}}{V\times\hat{B}\times V^{\dagger}}\times V\times\hat{I}\times V^{\dagger}\\ &=\frac{\hat{A}^{>}}{\hat{B}^{>}}\times\hat{I}^{>}=\hat{A}^{>}\,\hat{\div}^{>}\,\hat{B}^{>} \qquad (15)\end{aligned}$$

or alternatively,

$$\begin{aligned}\hat{A}\hat{\div}\hat{B} \quad \longrightarrow \quad & V\times(\hat{A}\hat{\div}\hat{B})\times V^{\dagger}=V\times(\hat{A}(\div\times\hat{I})\hat{B})\times V^{\dagger}\\ &=\Big((V\times\hat{A}\times V^{\dagger})\div(V\times\hat{B}\times V^{\dagger})\Big)\times V\times\hat{I}\times V^{\dagger}\\ &=\hat{A}^{>}\,\hat{\div}^{>}\,\hat{B}^{>} \qquad (16)\end{aligned}$$

That means we have for *genotopic division*,

$$\hat{\div}^{>}=\div\times\hat{I}^{>},\quad \hat{/}^{>}=(/)\times\hat{I}^{>} \qquad (17)$$

and

$${}^{<}\hat{\div}={}^{<}\hat{I}\times\div,\quad {}^{<}\hat{/}={}^{<}\hat{I}\times(/) \qquad (18)$$

Other aspects of the considered genotopy are:

- The broader genomathematics is then given by: The lifting of isofields $\hat{F}(\hat{a},\,\hat{+},\,\hat{x})$ into the *forward and backward geno-fields* $\hat{F}^{>}(\hat{a}^{>},\,\hat{+}^{>},\,>)$ and ${}^{<}\hat{F}({}^{<}\hat{c},\,{}^{<}\hat{+},\,<)$ with *forward and backward genonumbers* $\hat{a}^{>}=a\times\hat{I}^{>}$ and ${}^{<}\hat{a}={}^{<}\hat{I}\times a$, and related operations [33].

- The lifting of isofunctions $\hat{f}(\hat{r})$ on $\hat{F}$ into the *forward and backward genofunctions* $\hat{f}^{>}(\hat{r}^{>})$ and ${}^{<}\hat{f}({}^{<}\hat{r})$ on $\hat{F}^{>}$ and ${}^{<}\hat{F}$, respectively, such as $(\hat{e}^{>})^{\hat{X}^{>}}=\left(e^{\hat{X}^{>}\times\hat{S}}\right)\times\hat{I}^{>}$ and ${}^{<}\hat{e}^{{}^{<}\hat{X}}={}^{<}\hat{I}\times e^{\hat{R}\times{}^{<}\hat{X}}$, with consequential genotopies of transforms and functional analysis at large [4].

- The lifting of the *isodifferential calculus* into the *forward and backward genodifferential calculus* with main forward rules $\hat{d}^{>}\hat{r}^{>k}=\hat{I}_{i}^{>k}\times$

$\hat{d}^{>i}\hat{r}^{>i}$, $\hat{d}^{>}\hat{p}_k^{>} = \hat{S}_k^{>i} \times d\hat{p}_i^{>}$, $\hat{\partial}^{>}/\hat{\partial}^{>}\hat{r}^{>i} = \hat{S}_i^{>j} \times \partial/\partial\hat{r}^{>j}$, $\hat{\partial}^{>}/\hat{\partial}^{>}\hat{p}_k^{>} = \hat{S}_k^{>i} \times \partial/\partial\hat{p}_i^{>}$, $\hat{\partial}^{>}\hat{r}^{>i}/\hat{\partial}^{>}\hat{r}^{>j} = \hat{\delta}_j^{>i} = \delta_j^i \times \hat{I}^{>}$, etc., and corresponding backward rules easily obtainable via conjugation [34].

- The lifting of isotopologies, isogeometries, etc. into the dual forward and backward genotopic forms.

5 Some of the examples of geno-equations

Some of the representative geno-equations are:

- *Forward Newton-Santilli genoequation for matter* [4]:

$$\hat{m}_a^{>} > \frac{\hat{d}^{>}\hat{v}_{ak}^{>}}{\hat{d}^{>}\hat{t}^{>}} = -\frac{\hat{\partial}^{>}\hat{V}^{>}(\hat{r})}{\hat{\partial}^{>}\hat{r}_{ak}^{>}}, \tag{19}$$

- *Geno-internal energy balance equation* [29, 35]:

$$\rho^{>} > \frac{d^{>}u^{>}}{d^{>}t^{>}} = -\nabla^{>} \odot^{>} \mathbf{q}^{>} - p^{>} > \rho^{>} > \frac{d^{>}v^{>}}{d^{>}t^{>}} + \mathbf{\Pi}^{>} \odot^{>} \nabla^{>}\mathbf{u}^{>} \tag{20}$$

- *Geno-Clausius Inequality for closed systems* [29, 35]:

$$\oint^{>} \frac{d^{>}Q^{>}}{T_R} < 0 \qquad \text{(closed systems)} \tag{21}$$

- *Geno-Clausius Inequality for a temperature field on the bounding surface of the closed system* [29, 35]:

$$\oint^{>} \left[\frac{1^{>}}{T_{_R}} > \frac{d^{>}Q^{>}}{d^{>}t^{>}}\right] > d^{>}t^{>}$$
$$\equiv \oint^{>} \left[\int_{A^{>}}^{>} -\frac{\mathbf{Q}^{>}(\mathbf{A}^{>})}{T^{>}(\mathbf{A}^{>})} \odot^{>} \mathbf{d}^{>}\mathbf{A}^{>}\right] > d^{>}t^{>} < 0 \quad \text{(closed systems)} \tag{22}$$

6 Concluding remarks

We have seen that thermodynamic reversibility is uniquely determined. Though the thermodynamic forward and reversed paths are not real ones but it guarantees assuming of the same equilibrium states in reverse order on the said reversed path. Of course the equilibrium states are real ones. The same is not possible with dynamical equations because herein there exists an additional parameter of time. However, the explicit existence of time parameter offers a possibility to test the dynamic equations for *time reversal symmetry*. Thus the time reversal symmetry and the thermodynamic reversibility are determined entirely on two different footings.

We have seen that even if a dynamical equation is symmetric to time reversal the reversed path are not obtained as composed of the same dynamic states. This is so because the reversal of time reverses velocity vector and hence the dynamic states are not identically same as those encountered on the forward path. Thus in the case of symmetric to time reversal dynamical equations what one obtains is the spatial reversibility. Hence it is a partial description of reversibility and there is no physical utility of this test. Therefore, even if an equation of motion is symmetric to time reversal the forward and reverse paths it describe are two different irreversible motions.

Further, from the physical utility point of view those equations not found symmetric to time reversal produce additional ambiguities. For example, whether the sign of say momentum flux changes on time reversal or not remains an unanswered or ambiguously answered question. Hence, what happens to the corresponding dissipative term on time reversal cannot be predicted uniquely. This also has repercussions even on the validity of the second law of thermodynamics on the time reversed paths. Recall that thermodynamic irreversibility is determined by the existence of entropy source strength with positive definite sign and hence it is termed as entropy production. Because of the above we get caught into a trap that suggest that even the thermodynamic irreversibility doesn't get properly described on a time reversed path. That is thermodynamic irreversibility is at the verge of loosing sanctity on time reversed paths. Such results remain unacceptable.

We are astonished to see that whether the Boltzmann integro-differential equation is symmetric to time reversal or not, the Boltzmann H-theorem

remains time reversal invariant. However, this result is conventionally taken as the kinetic theory given second law of thermodynamics.

Most importantly we need to keep in mind is that the time reversal test we perform on the equations of motion and not on the actual motion. All actual motions are inherently irreversible whether the equation used to describe them are symmetric to time reversal or not. Mathematical description of motions that produce ambiguous results on time reversal operation are also inherently irreversible.

Thus the time reversal test is of no practical utility particularly in better understanding of either dynamic irreversibility or thermodynamic irreversibility. Therefore, we conclude that the mathematics of 20^{th} century and the mechanics based on it are not compatible with the real physical motions. Hence, one needs to use a mathematics which is inherently irreversible to describe dynamics of all real motions and also to develop nonequilibrium thermodynamics.

The above requirement is perfectly met by Santilli's genomathematics and the mechanics based on it. This is so because herein one uses two different multiplying units $\hat{I}^{>}$ and ${}^{<}\hat{I}$ for forward and backward motions with $\hat{I}^{>} \neq {}^{<}\hat{I}$. Hence, there is no requirement of testing time reversal symmetry of equations.

Thus we safely conclude that there is no other option than the Lie-admissible mathematics (genomathematics) of Santilli commensurate with the irreversible motion and nonequilibrium thermodynamics [7].

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